

STN

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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 10	Time limit for inactive STN sessions doubles to 40 minutes
NEWS	3	AUG 18	COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS	4	AUG 24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS	5	AUG 24	CA/CAplus enhanced with legal status information for U.S. patents
NEWS	6	SEP 09	50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS	7	SEP 11	WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus
NEWS	8	OCT 21	Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded
NEWS	9	OCT 21	Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models
NEWS	10	OCT 27	Free display of legal status information in CA/CAplus, USPATFULL, and USPAT2 in the month of November.

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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FILE 'HOME' ENTERED AT 19:20:54 ON 05 NOV 2009

STN

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=> file reg
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY        SESSION
FULL ESTIMATED COST          0.22          0.22
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FILE 'REGISTRY' ENTERED AT 19:21:02 ON 05 NOV 2009
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STRUCTURE FILE UPDATES: 4 NOV 2009 HIGHEST RN 1191231-18-1
DICTIONARY FILE UPDATES: 4 NOV 2009 HIGHEST RN 1191231-18-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

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L1 STRUCTURE UPLOADED

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=> s 11
L2      759 1L
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=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 19:23:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 533879 TO ITERATE
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100.0% PROCESSED 533879 ITERATIONS 1677 ANSWERS
SEARCH TIME: 00.00.16

L3 1677 SEA SSS FUL L1

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=> file hcaplus
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FILE 'HCAPLUS' ENTERED AT 19:24:12 ON 05 NOV 2009
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FILE COVERS 1907 - 5 Nov 2009 VOL 151 ISS 19
FILE LAST UPDATED: 4 Nov 2009 (20091104/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

HCplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

During November, try the new LSUS format of legal status information in the CA/CAplus family databases for free! Complete details on the number of free displays and other databases participating in this offer appear in NEWS 10.

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=> s 13
L4      376 L3

=> s 13/uses
      376 L3
      7822042 USES/RL
L5      58 L3/USES
      (L3 (L) USES/RL)

=> s 14 and trotter, b?/au
      56 TROTTER, B?/AU
L6      4 L4 AND TROTTER, B?/AU

=> d 16, ibib abs hitstr, 1-4
THE ESTIMATED COST FOR THIS REQUEST IS 22.56 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L6 ANSWER 1 OF 4 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1252121 HCPLUS
DOCUMENT NUMBER: 146:142484
TITLE: Design and Synthesis of Novel Isoquinoline-3-nitriles
       as Orally Bioavailable Kv1.5 Antagonists for the
```

STN

AUTHOR(S): Treatment of Atrial Fibrillation
Trotter, B. Wesley; Nanda, Kausik K.; Kett, Nathan R.; Regan, Christopher P.; Lynch, Joseph J.; Stump, Gary L.; Kiss, Laszlo; Wang, Jixin; Spencer, Robert H.; Kane, Stefanie A.; White, Rebecca B.; Zhang, Rena; Anderson, Kenneth D.; Liverton, Nigel J.; McIntyre, Charles J.; Beshore, Douglas C.; Hartman, George D.; Dinsmore, Christopher J.

CORPORATE SOURCE: Departments of Medicinal Chemistry, Stroke, and Neurodegeneration Automated Biotechnology Pain Research, and Drug Metabolism, Merck Research Laboratories, West Point, PA, 19486, USA

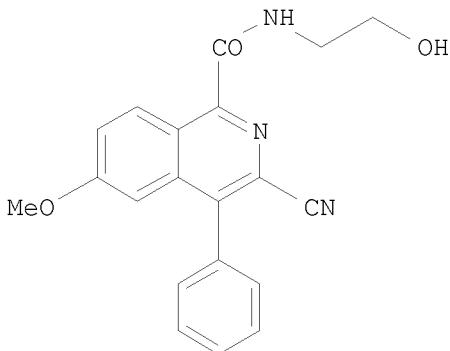
SOURCE: Journal of Medicinal Chemistry (2006), 49(24), 6954-6957
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:142484
GI



AB Novel 3-cyanoisoquinoline Kv1.5 antagonists have been prepared and evaluated in in vitro and in vivo assays for inhibition of the Kv1.5 potassium channel and its associated cardiac potassium current, IKur. Structural modifications of the isoquinolinone lead afforded compds. (e.g. I) with excellent potency, selectivity, and oral bioavailability.

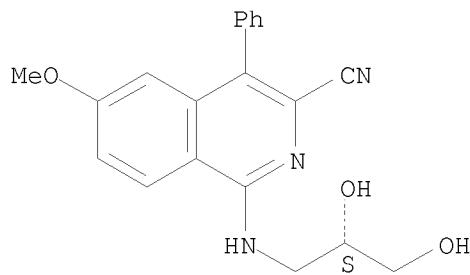
IT 849546-23-2P 849546-30-1P 849547-28-0P
849548-50-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of isoquinoline-3-nitriles as orally bioavailable Kv1.5 antagonists for the treatment of atrial fibrillation)

RN 849546-23-2 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-2,3-dihydroxypropyl]amino]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

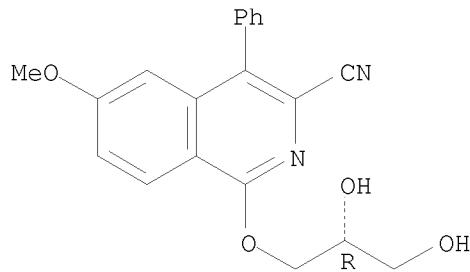
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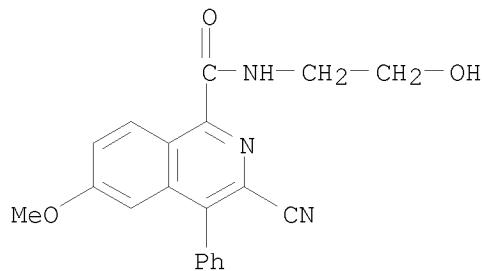
CN 3-Isoquinolinecarbonitrile, 1-[(2R)-2,3-dihydroxypropoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 849547-28-0 HCAPLUS

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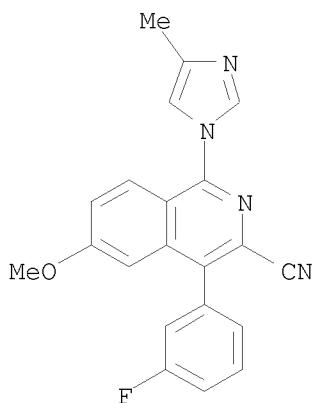


RN 849548-50-1 HCAPLUS

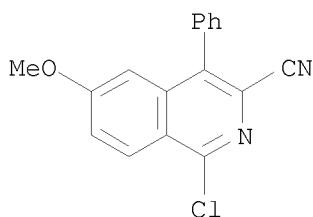
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(4-methyl-1H-imidazol-1-yl)- (CA INDEX NAME)

Updated Search

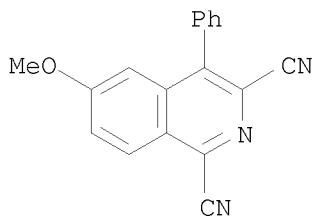
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IT 849546-10-7P 849546-11-8P 849546-26-5P
849546-48-1P 849547-30-4P 849549-26-4P
849549-27-5P, 4-(3-Fluorophenyl)-6-methoxy-1-oxo-1,2-
dihydroisoquinoline-3-carbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of isoquinoline-3-nitriles as orally bioavailable Kv1.5
antagonists for the treatment of atrial fibrillation)
RN 849546-10-7 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 1-chloro-6-methoxy-4-phenyl- (CA INDEX NAME)



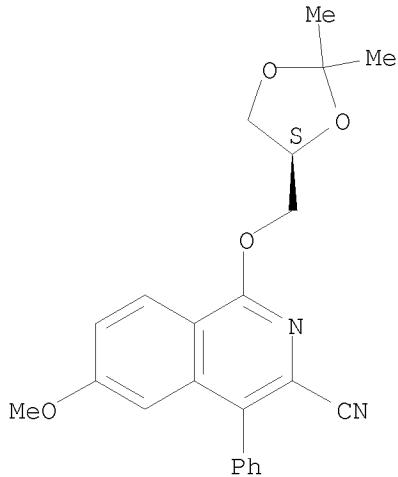
RN 849546-11-8 HCPLUS
CN 1,3-Isoquinolinedicarbonitrile, 6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849546-26-5 HCAPLUS
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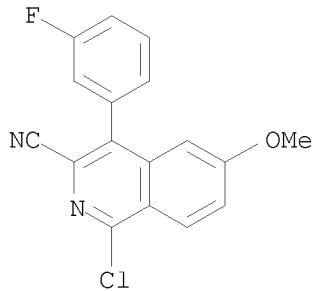
STN

Absolute stereochemistry.



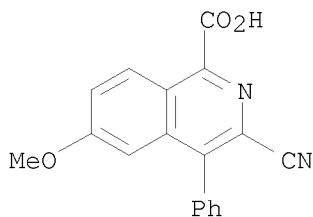
RN 849546-48-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-chloro-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849547-30-4 HCAPLUS

CN 1-Isoquinolinecarboxylic acid, 3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)

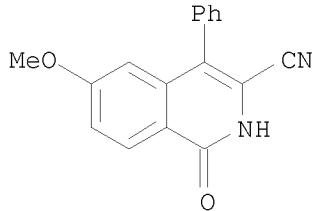


RN 849549-26-4 HCAPLUS

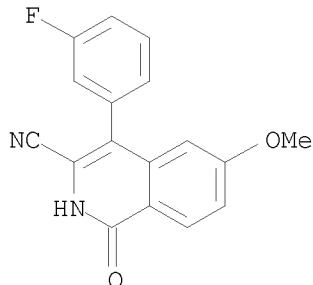
CN 3-Isoquinolinecarbonitrile, 1,2-dihydro-6-methoxy-1-oxo-4-phenyl- (CA INDEX NAME)

Updated Search

STN



RN 849549-27-5 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1,2-dihydro-6-methoxy-1-oxo-
(CA INDEX NAME)



OS.CITING REF COUNT: 29 THERE ARE 29 CAPLUS RECORDS THAT CITE THIS
RECORD (29 CITINGS)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:300465 HCAPLUS
DOCUMENT NUMBER: 142:373705
TITLE: Preparation of isoquinoline derivatives as potassium
channel inhibitors
INVENTOR(S): Trotter, B. Wesley; Claiborne, Christopher;
Ponticello, Gerald S.; McIntyre, Charles J.; Liverton,
Nigel; Claremon, David A.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

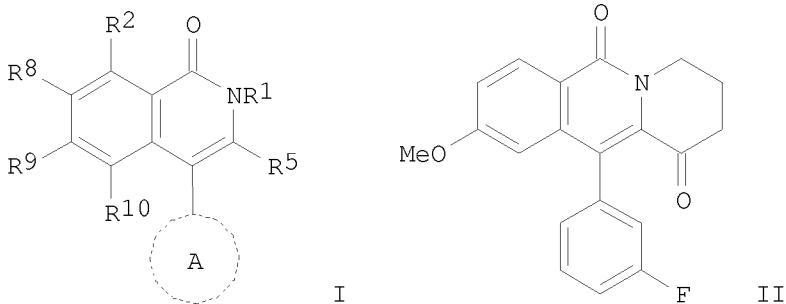
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030791	A2	20050407	WO 2004-US30431	20040917
WO 2005030791	A3	20050526		

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GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
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 SN, TD, TG

AU 2004276236	A1	20050407	AU 2004-276236	20040917
AU 2004276236	B2	20080124		
CA 2539814	A1	20050407	CA 2004-2539814	20040917
EP 1667982	A2	20060614	EP 2004-788811	20040917
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CN 1856476	A	20061101	CN 2004-80027369	20040917
JP 2007516218	T	20070621	JP 2006-528067	20040917
IN 2006DN01030	A	20070817	IN 2006-DN1030	20060227
US 20070027177	A1	20070201	US 2006-571870	20060315
PRIORITY APPLN. INFO.:			US 2003-505101P	P 20030923
			WO 2004-US30431	W 20040917

OTHER SOURCE(S): CASREACT 142:373705; MARPAT 142:373705
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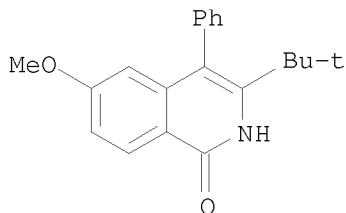


AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl; R1 = H, (cyclo)alkyl, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbamoyl, etc.; R5 = H, halo, (cyclo)alkyl, etc.; or R1R5 = (un)substituted cyclic ring; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, reaction of 2-(3-fluorobenzoyl)-4-methoxybenzoyl chloride with piperidin-3-one•HCl gave II. I provide ≥20 % inhibition at a concentration of 33 μM or less in the high throughput Kv1.5 planar patch clamp assay and ≥25 % inhibition at a concentration of 25 μM or less in the AAS (Atomic Absorption Spectroscopy) assay. Thus, I and their pharmaceutical compns. are useful as potassium channel inhibitors for the treatment of cardiac arrhythmias, and the like.

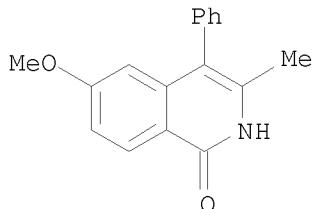
IT 849424-93-7P 849424-95-9P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

STN

(preparation of isoquinoline derivs. as potassium channel inhibitors)
RN 849424-93-7 HCAPLUS
CN 1(2H)-Isoquinolinone, 3-(1,1-dimethylethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849424-95-9 HCAPLUS
CN 1(2H)-Isoquinolinone, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

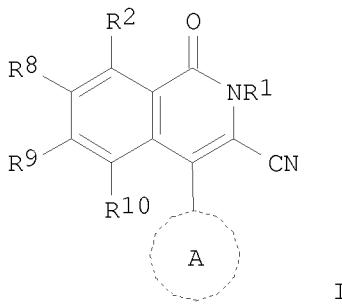
L6 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:300412 HCAPLUS
DOCUMENT NUMBER: 142:373702
TITLE: Preparation of isoquinoline derivatives as potassium
channel inhibitors
INVENTOR(S): Isaacs, Richard; Dinsmore, Christopher J.;
Trotter, B. Wesley; Liverton, Nigel; Beshore,
Douglas C.; Kett, Nathan R.; McIntyre, Charles J.;
Nanda, Kausik K.; Claremon, David A.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030729	A1	20050407	WO 2004-US30945	20040922
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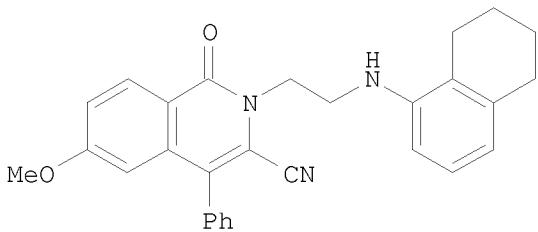
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 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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AU 2004276268	A1	20050407	AU 2004-276268	20040922
AU 2004276268	B2	20090129		
CA 2539546	A1	20050407	CA 2004-2539546	20040922
EP 1667981	A1	20060614	EP 2004-784700	20040922
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JP 2007506749	T	20070322	JP 2006-528111	20040922
US 20070054892	A1	20070308	US 2006-572236	20060317
IN 2006DN01544	A	20070810	IN 2006-DN1544	20060322
PRIORITY APPLN. INFO.:			US 2003-505216P	P 20030923
			WO 2004-US30945	W 20040922

OTHER SOURCE(S): CASREACT 142:373702; MARPAT 142:373702
 GI



I



II

AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl; R1 = H, (cyclo)alkyl, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbamoyl, etc.; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, II was given in a multi-step synthesis starting from the reaction of p-anisoyl chloride with aniline. I provide ≥20 % inhibition at a concentration of 33 μM or

STN

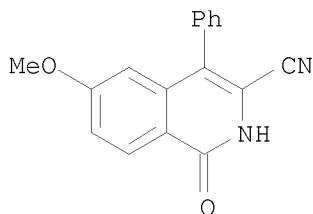
less in the high throughput Kv1.5 planar patch clamp assay and ≥ 25 % inhibition at a concentration of 25 μM or less in the AAS (Atomic Absorption Spectroscopy) assay. Thus, I and their pharmaceutical compns. are useful as potassium channel inhibitors for the treatment of cardiac arrhythmias, and the like.

IT 849549-26-4P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849549-26-4 HCPLUS

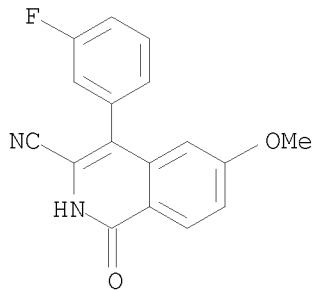
CN 3-Isoquinolinecarbonitrile, 1,2-dihydro-6-methoxy-1-oxo-4-phenyl- (CA INDEX NAME)



IT 849549-27-5P, 4-(3-Fluorophenyl)-6-methoxy-1-oxo-1,2-dihydroisoquinoline-3-carbonitrile 849549-29-7P,
4-(2-Fluorophenyl)-6-methoxy-1-oxo-1,2-dihydroisoquinoline-3-carbonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849549-27-5 HCPLUS

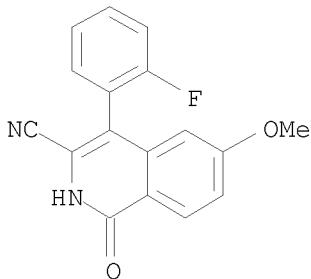
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1,2-dihydro-6-methoxy-1-oxo- (CA INDEX NAME)



RN 849549-29-7 HCPLUS

CN 3-Isoquinolinecarbonitrile, 4-(2-fluorophenyl)-1,2-dihydro-6-methoxy-1-oxo- (CA INDEX NAME)

STN

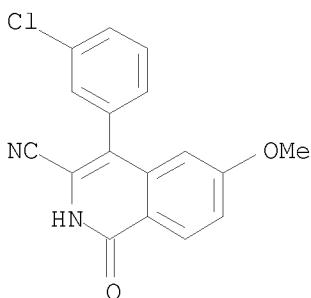


IT 849635-33-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849635-33-2 HCPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1,2-dihydro-6-methoxy-1-oxo-
(CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:300191 HCPLUS

DOCUMENT NUMBER: 142:373697

TITLE: Preparation of isoquinoline derivatives as potassium
channel inhibitors

INVENTOR(S): Trotter, B. Wesley; Nanda, Kausik K.; Kett,
Nathan R.; Dinsmore, Christopher J.; Ponticello,
Gerald S.; Claremon, David A.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 115 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND DATE

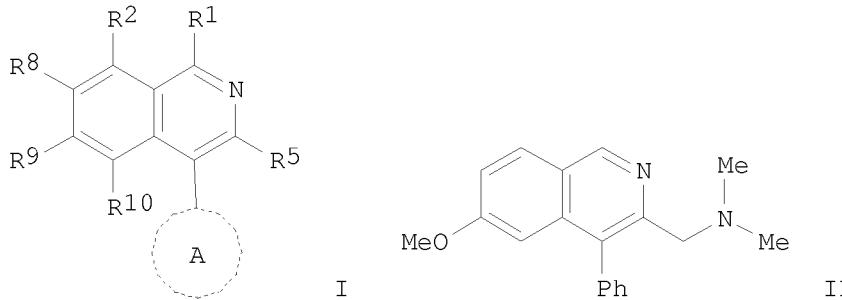
APPLICATION NO.

DATE

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AU 2004275720	B2	20080424		
CA 2539479	A1	20050407	CA 2004-2539479	20040917
EP 1667979	A2	20060614	EP 2004-784370	20040917
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CN 1856475	A	20061101	CN 2004-80027385	20040917
JP 2007506743	T	20070322	JP 2006-528072	20040917
IN 2006DN00877	A	20070810	IN 2006-DN877	20060220
US 20060276450	A1	20061207	US 2006-572342	20060317
PRIORITY APPLN. INFO.:			US 2003-505143P	P 20030923
			WO 2004-US30486	W 20040917

OTHER SOURCE(S): CASREACT 142:373697; MARPAT 142:373697

GI



AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl or heterocyclic ring; R1 = H, CN, halo, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbamoyl, etc.; R5 = H, halo, (cyclo)alkyl, etc.; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, Ni-catalyzed reduction of 1-chloro-6-methoxy-4-phenylisoquinoline-3-carbonitrile and followed by condensation with formaldehyde, gave II•2HCl. I provided ≥50% inhibition at concentration ≤33 μM in the high-throughput Kv1.5 planar patch clamp assay and ≥25% inhibition at concentration ≤25 μM in the AAS (atomic absorption spectroscopy) assay. Thus, I and their pharmaceutical compns. are useful as potassium channel inhibitors for the

STN

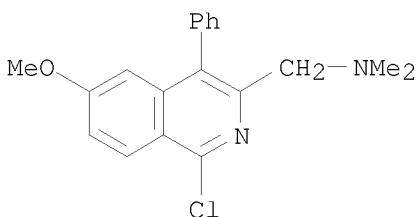
treatment of cardiac arrhythmias, and the like.

IT 849545-74-0P 849545-76-2P 849546-10-7P
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849546-26-5P 849546-28-7P 849546-48-1P
849546-58-3P 849547-30-4P 849548-92-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of isoquinoline derivs. as potassium channel inhibitors)

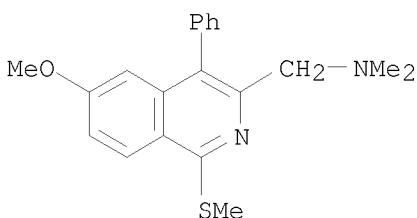
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CN 3-Isoquinolinemethanamine, 1-chloro-6-methoxy-N,N-dimethyl-4-phenyl- (CA INDEX NAME)



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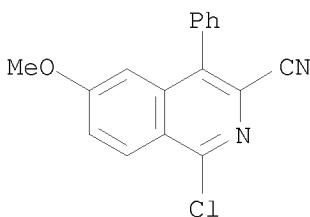
CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-1-(methylthio)-4-phenyl-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

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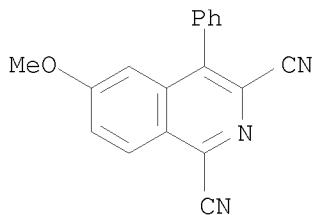
CN 3-Isoquinolinecarbonitrile, 1-chloro-6-methoxy-4-phenyl- (CA INDEX NAME)



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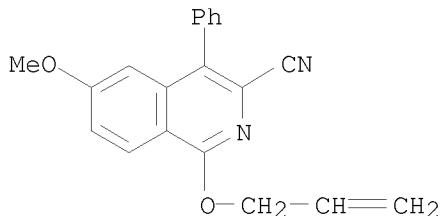
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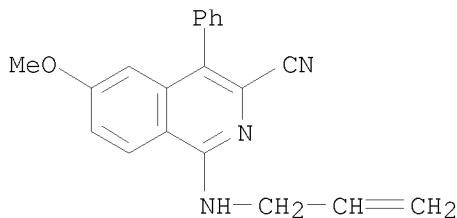
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CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-(2-propen-1-yloxy)- (CA INDEX NAME)



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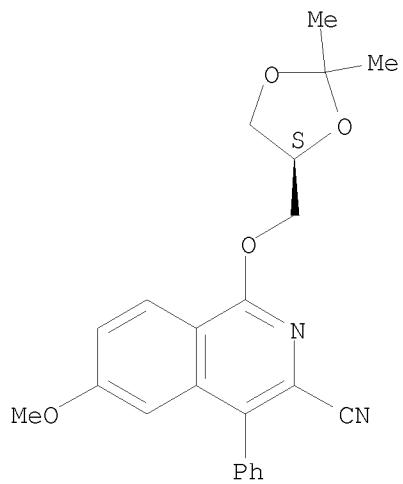


RN 849546-26-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(4S)-2,2-dimethyl-1,3-dioxolan-4-yl]methoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

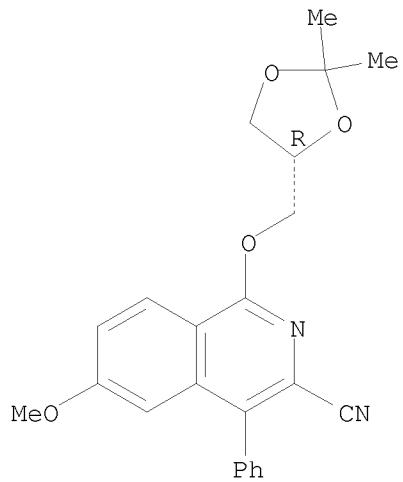
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RN 849546-28-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(4R)-2,2-dimethyl-1,3-dioxolan-4-yl]methoxy-4-phenyl- (CA INDEX NAME)

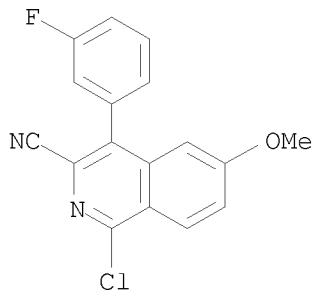
Absolute stereochemistry.



RN 849546-48-1 HCAPLUS

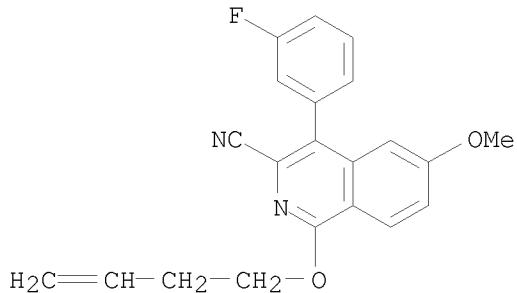
CN 3-Isoquinolinecarbonitrile, 1-chloro-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

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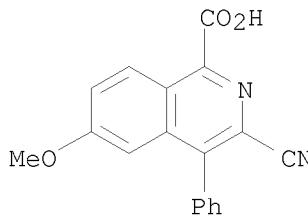
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CN 3-Isoquinolinecarbonitrile, 1-(3-buten-1-yloxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



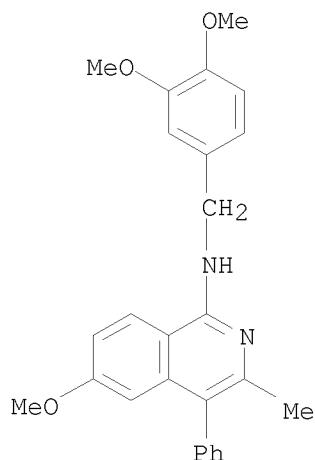
RN 849547-30-4 HCAPLUS

CN 1-Isoquinolinecarboxylic acid, 3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849548-92-1 HCAPLUS

CN 1-Isoquinolinamine, N-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



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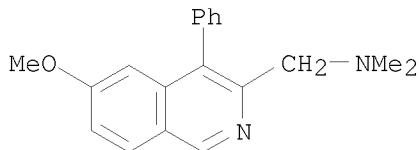
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849545-72-8 HCPLUS

CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-4-phenyl-, hydrochloride (1:2) (CA INDEX NAME)

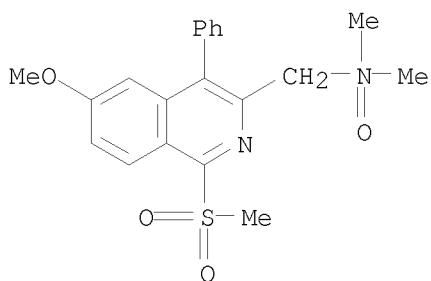


●2 HCl1

RN 849545-78-4 HCPLUS

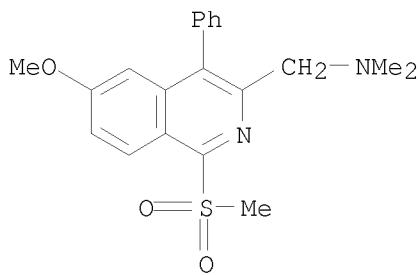
CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-1-(methylsulfonyl)-4-phenyl-, N-oxide (CA INDEX NAME)

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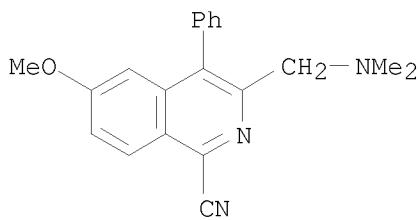
RN 849545-80-8 HCAPLUS

CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-1-(methylsulfonyl)-4-phenyl- (CA INDEX NAME)



RN 849545-82-0 HCAPLUS

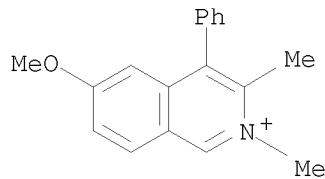
CN 1-Isoquinolinecarbonitrile, 3-[(dimethylamino)methyl]-6-methoxy-4-phenyl-
(CA INDEX NAME)



RN 849545-84-2 HCAPLUS

CN Isoquinolinium, 6-methoxy-2,3-dimethyl-4-phenyl-, hydroxide (1:1) (CA INDEX NAME)

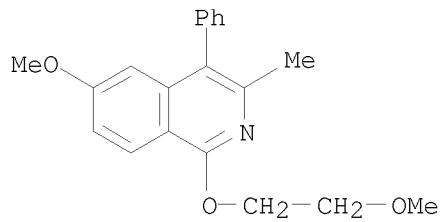
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● OH⁻

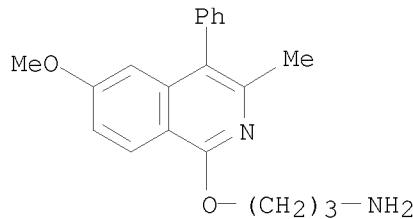
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CN Isoquinoline, 6-methoxy-1-(2-methoxyethoxy)-3-methyl-4-phenyl- (CA INDEX NAME)



RN 849545-88-6 HCAPLUS

CN 1-Propanamine, 3-[(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)oxy]-, hydrochloride (1:2) (CA INDEX NAME)

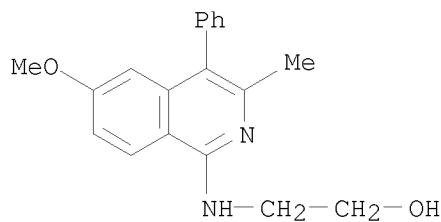


●2 HCl

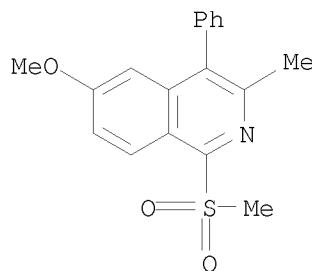
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CN Ethanol, 2-[(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)amino]- (CA INDEX NAME)

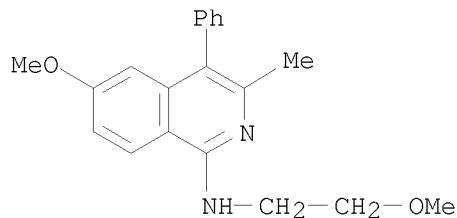
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RN 849545-91-1 HCAPLUS
CN Isoquinoline, 6-methoxy-3-methyl-1-(methylsulfonyl)-4-phenyl- (CA INDEX NAME)



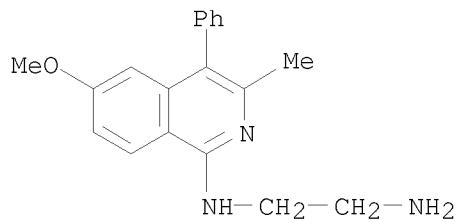
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CN 1-Isoquinolinamine, 6-methoxy-N-(2-methoxyethyl)-3-methyl-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

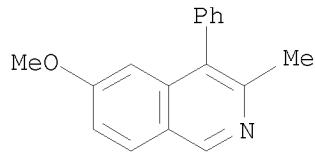
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CN 1,2-Ethanediamine, N1-(6-methoxy-3-methyl-4-phenyl-1-isooquinolinyl)-, hydrochloride (1:2) (CA INDEX NAME)

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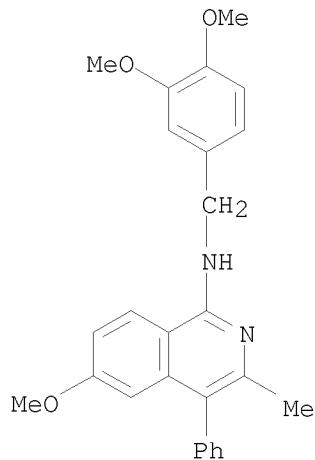
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RN 849545-95-5 HCPLUS
CN Isoquinoline, 6-methoxy-3-methyl-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 849545-97-7 HCPLUS
CN 1-Isoquinolinamine, N-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-3-methyl-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



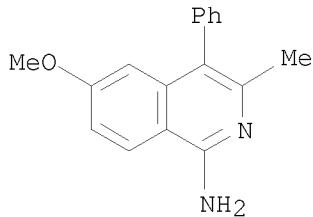
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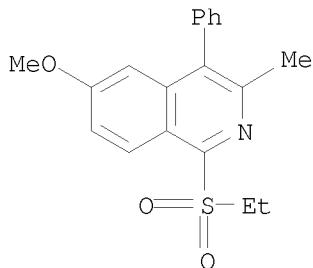
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CN 1-Isoquinolinamine, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



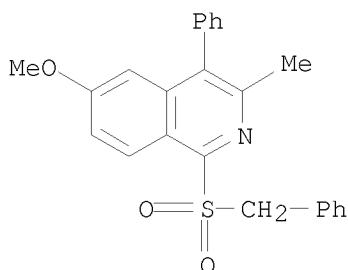
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CN Isoquinoline, 1-(ethylsulfonyl)-6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



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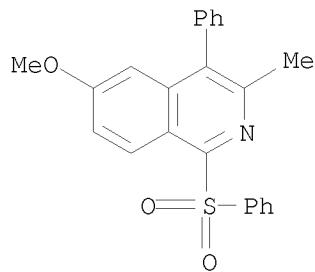
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RN 849546-04-9 HCAPLUS

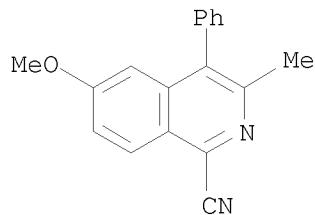
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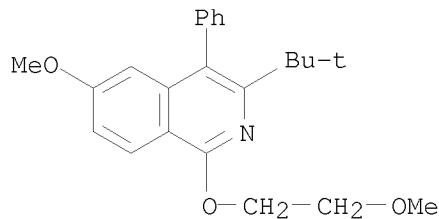
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CN 1-Isoquinolinecarbonitrile, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



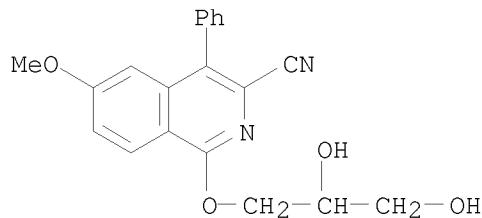
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CN Isoquinoline, 3-(1,1-dimethylethyl)-6-methoxy-1-(2-methoxyethoxy)-4-phenyl- (CA INDEX NAME)



RN 849546-15-2 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-(2,3-dihydroxypropoxy)-6-methoxy-4-phenyl- (CA INDEX NAME)

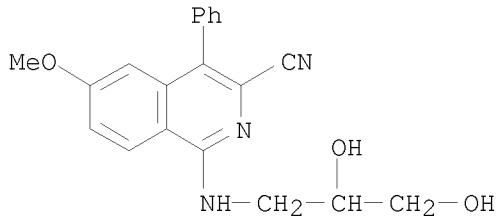


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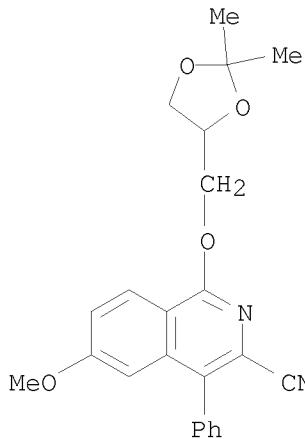
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CN 3-Isoquinolinecarbonitrile, 1-[(2,3-dihydroxypropyl)amino]-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849546-21-0 HCPLUS

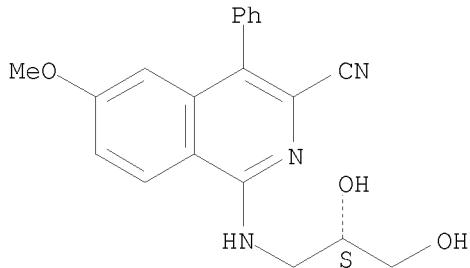
CN 3-Isoquinolinecarbonitrile, 1-[(2,2-dimethyl-1,3-dioxolan-4-yl)methoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849546-23-2 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-2,3-dihydroxypropyl]amino]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

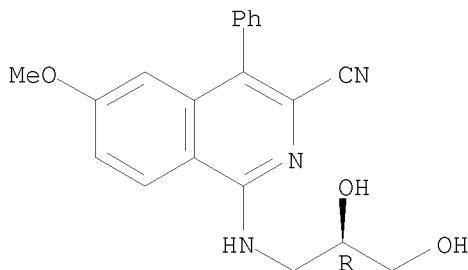


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RN 849546-25-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2R)-2,3-dihydroxypropyl]amino]-6-methoxy-4-phenyl- (CA INDEX NAME)

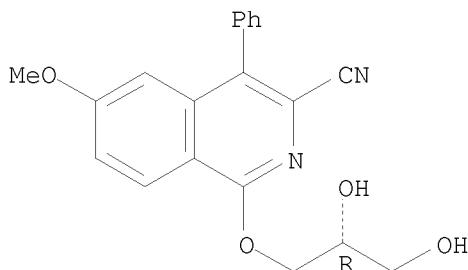
Absolute stereochemistry.



RN 849546-30-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2R)-2,3-dihydroxypropoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)

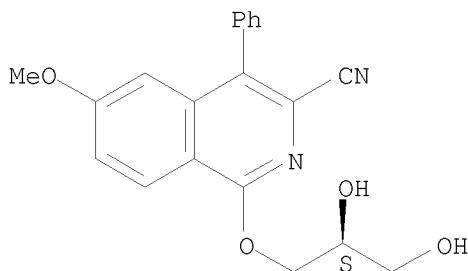
Absolute stereochemistry.



RN 849546-32-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-2,3-dihydroxypropoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



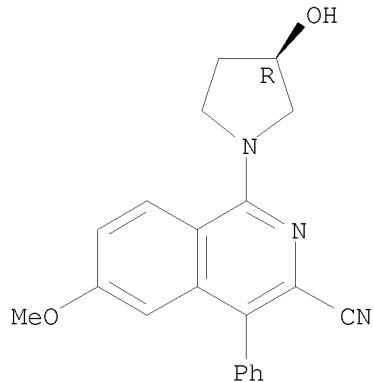
RN 849546-34-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3R)-3-hydroxy-1-pyrrolidinyl]-6-methoxy-4-

STN

phenyl- (CA INDEX NAME)

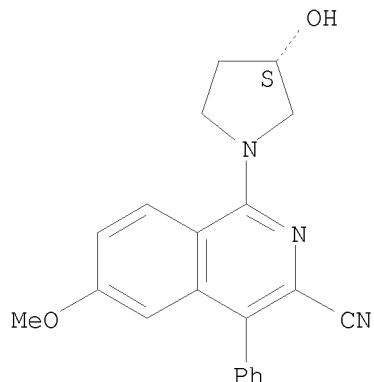
Absolute stereochemistry.



RN 849546-36-7 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3S)-3-hydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

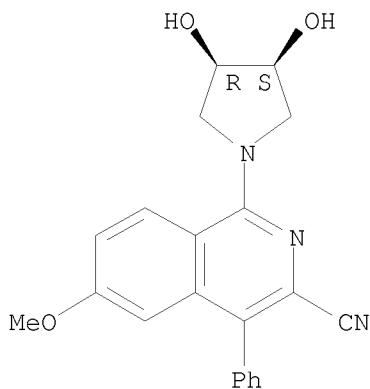


RN 849546-38-9 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3R,4S)-3,4-dihydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl-, rel- (CA INDEX NAME)

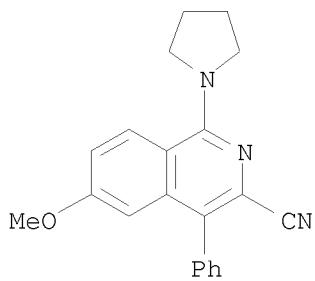
Relative stereochemistry.

STN



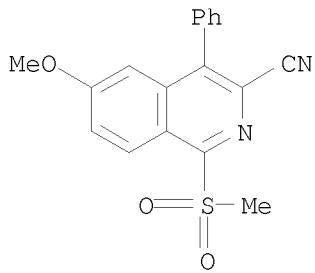
RN 849546-40-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-(1-pyrrolidinyl)- (CA INDEX NAME)



RN 849546-42-5 HCAPLUS

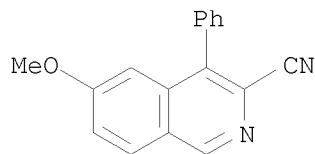
CN 3-Isoquinolinecarbonitrile, 6-methoxy-1-(methylsulfonyl)-4-phenyl- (CA INDEX NAME)



RN 849546-44-7 HCAPLUS

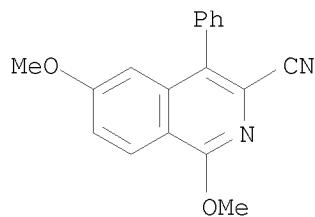
CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl- (CA INDEX NAME)

STN



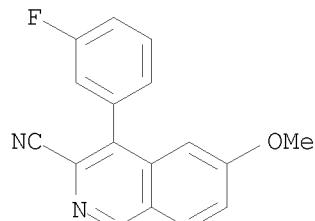
RN 849546-46-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1,6-dimethoxy-4-phenyl- (CA INDEX NAME)



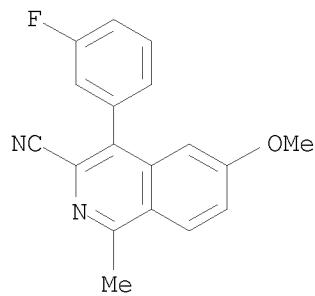
RN 849546-50-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849546-52-7 HCAPLUS

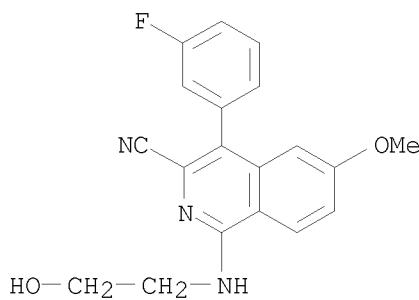
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-methyl- (CA INDEX NAME)



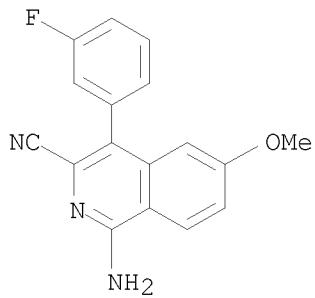
RN 849546-54-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-[(2-hydroxyethyl)amino]-6-methoxy- (CA INDEX NAME)

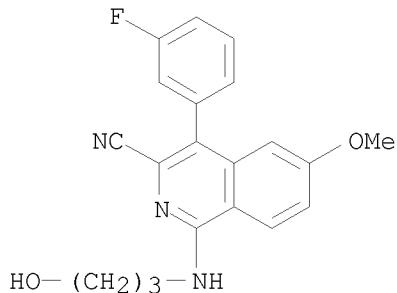
STN



RN 849546-56-1 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 1-amino-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

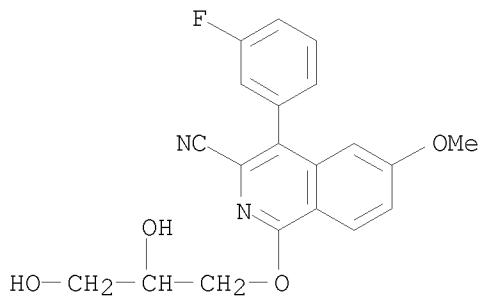


RN 849546-57-2 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-[(3-hydroxypropyl)amino]-6-methoxy- (CA INDEX NAME)



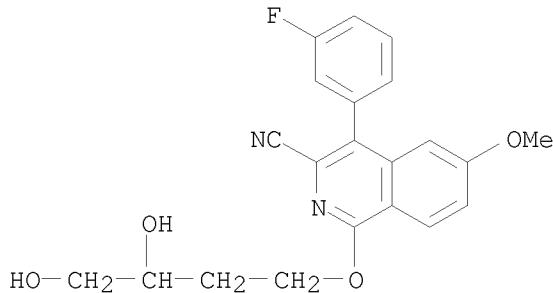
RN 849546-60-7 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 1-(2,3-dihydroxypropoxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

STN



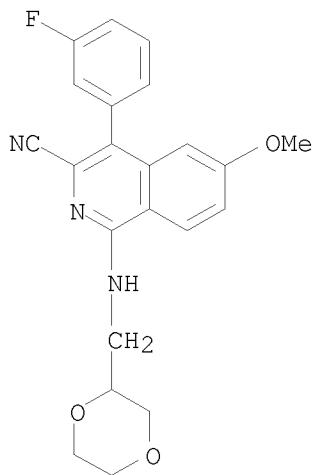
RN 849546-63-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(3,4-dihydroxybutoxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849546-66-3 HCAPLUS

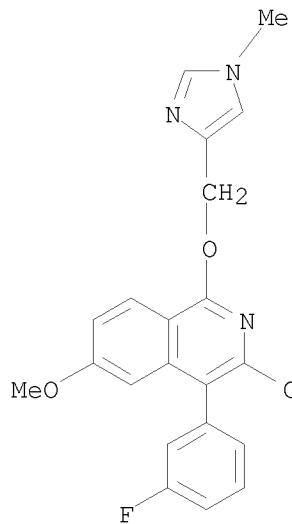
CN 3-Isoquinolinecarbonitrile, 1-[(1,4-dioxan-2-ylmethyl)amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849546-69-6 HCAPLUS

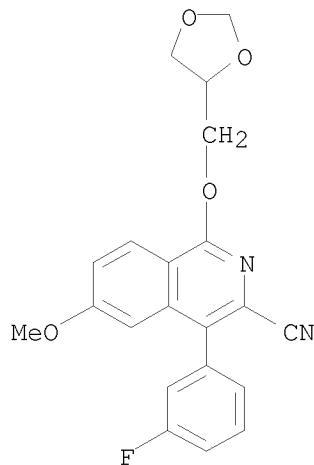
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-[(1-methyl-1H-imidazol-4-yl)methoxy]- (CA INDEX NAME)

STN



RN 849546-72-1 HCAPLUS

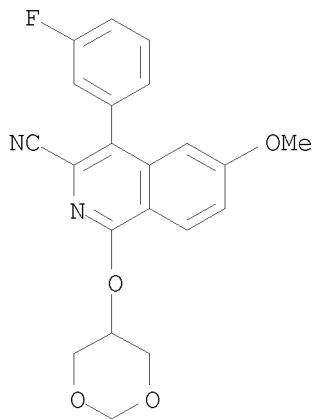
CN 3-Isoquinolinecarbonitrile, 1-(1,3-dioxolan-4-ylmethoxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849546-75-4 HCAPLUS

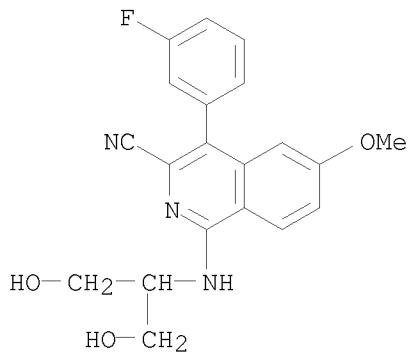
CN 3-Isoquinolinecarbonitrile, 1-(1,3-dioxan-5-ylmethoxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

STN



RN 849546-78-7 HCPLUS

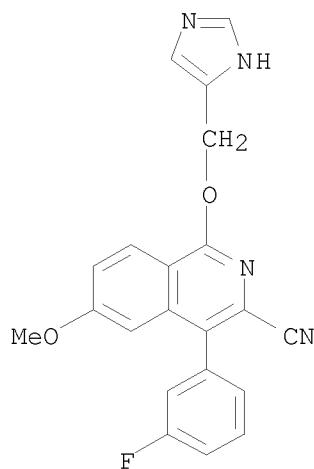
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-[2-hydroxy-1-(hydroxymethyl)ethyl]amino]-6-methoxy- (CA INDEX NAME)



RN 849546-80-1 HCPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-(1H-imidazol-5-ylmethoxy)-6-methoxy- (CA INDEX NAME)

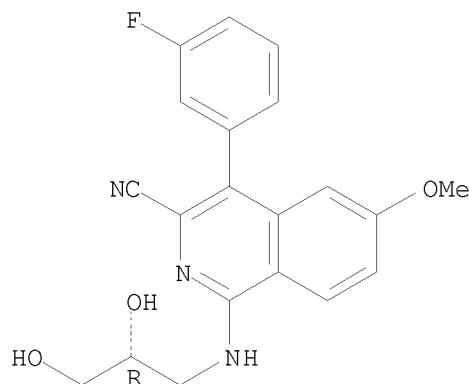
STN



RN 849546-83-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2R)-2,3-dihydroxypropyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

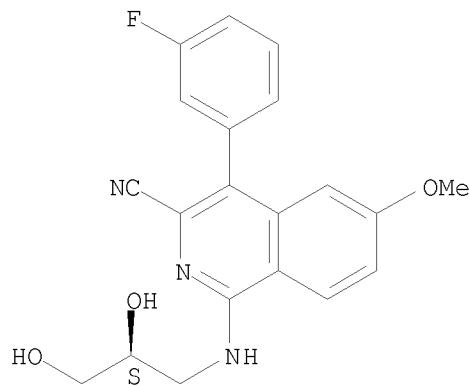


RN 849546-86-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-2,3-dihydroxypropyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

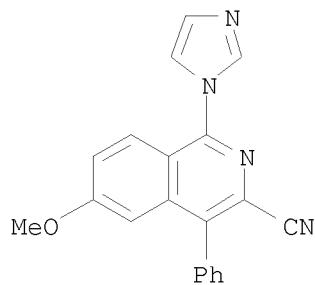
Absolute stereochemistry.

STN



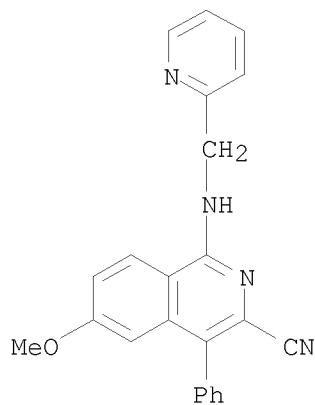
RN 849546-89-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(1H-imidazol-1-yl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849546-92-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-[(2-pyridinylmethyl)amino]- (CA INDEX NAME)

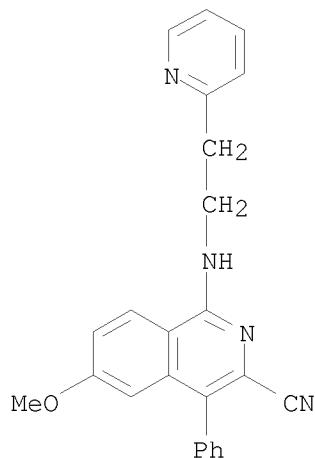


RN 849546-95-8 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-[(2-(2-

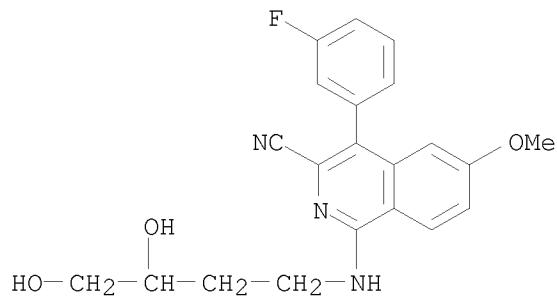
STN

pyridinyl)ethyl]amino]- (CA INDEX NAME)



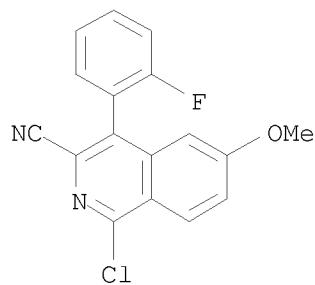
RN 849546-98-1 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3,4-dihydroxybutyl)amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849547-01-9 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-chloro-4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)

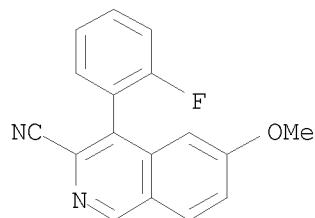


RN 849547-03-1 HCPLUS

Updated Search

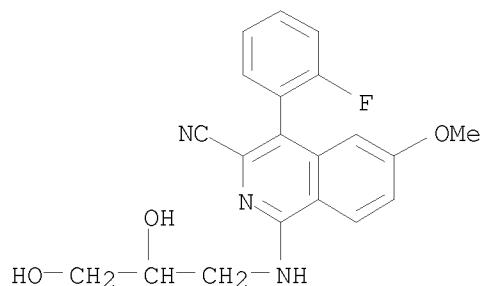
STN

CN 3-Isoquinolinecarbonitrile, 4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)



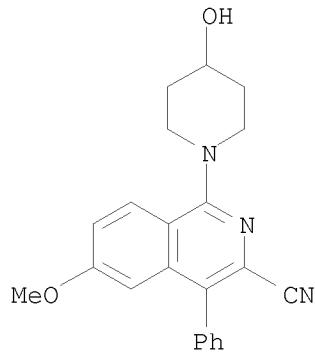
RN 849547-05-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2,3-dihydroxypropyl)amino]-4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849547-10-0 HCAPLUS

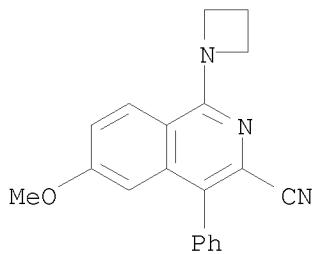
CN 3-Isoquinolinecarbonitrile, 1-(4-hydroxy-1-piperidinyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-13-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(1-azetidinyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

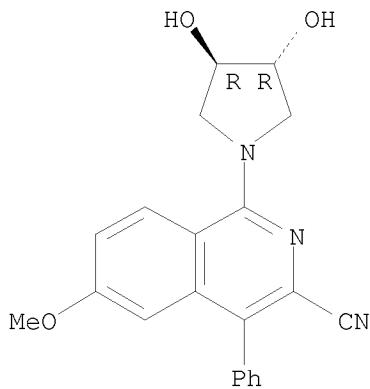
STN



RN 849547-15-5 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3R,4R)-3,4-dihydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

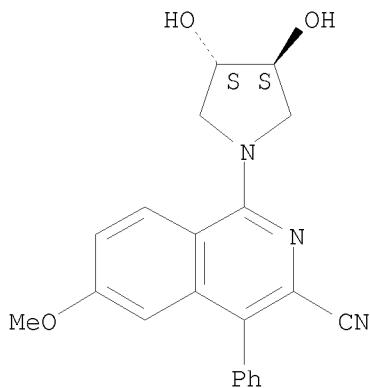
Absolute stereochemistry.



RN 849547-17-7 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3S,4S)-3,4-dihydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

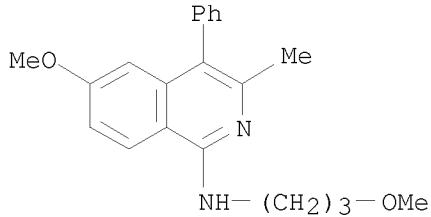


RN 849547-19-9 HCPLUS

Updated Search

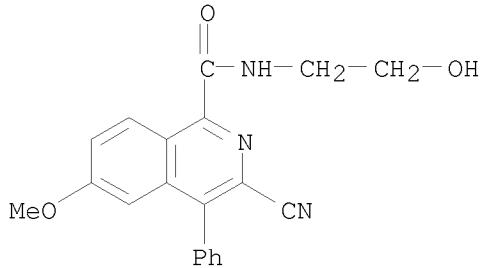
STN

CN 1-Isoquinolinamine, 6-methoxy-N-(3-methoxypropyl)-3-methyl-4-phenyl- (CA INDEX NAME)



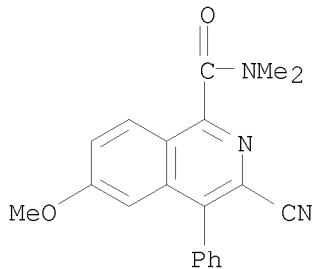
RN 849547-28-0 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-hydroxyethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-31-5 HCAPLUS

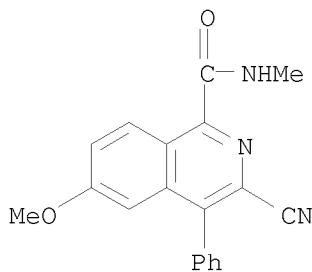
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N,N-dimethyl-4-phenyl- (CA INDEX NAME)



RN 849547-33-7 HCAPLUS

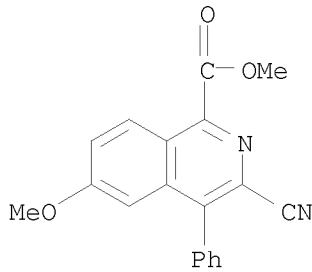
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-methyl-4-phenyl- (CA INDEX NAME)

STN



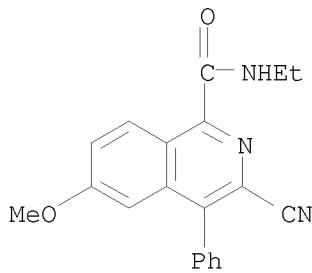
RN 849547-35-9 HCAPLUS

CN 1-Isoquinolinecarboxylic acid, 3-cyano-6-methoxy-4-phenyl-, methyl ester
(CA INDEX NAME)



RN 849547-37-1 HCAPLUS

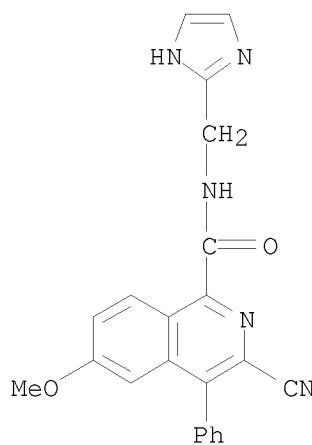
CN 1-Isoquinolinecarboxamide, 3-cyano-N-ethyl-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-39-3 HCAPLUS

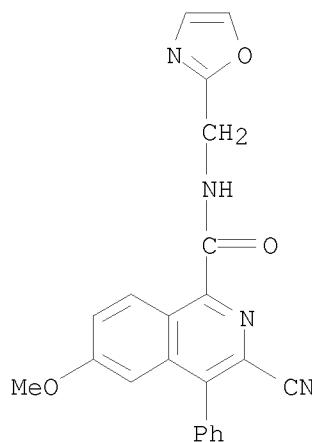
CN 1-Isoquinolinecarboxamide, 3-cyano-N-(1H-imidazol-2-ylmethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

STN



RN 849547-41-7 HCAPLUS

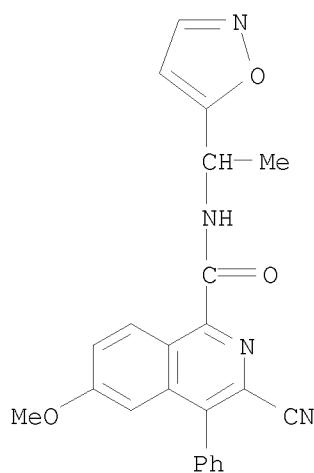
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-oxazolylmethyl)-4-phenyl-
(CA INDEX NAME)



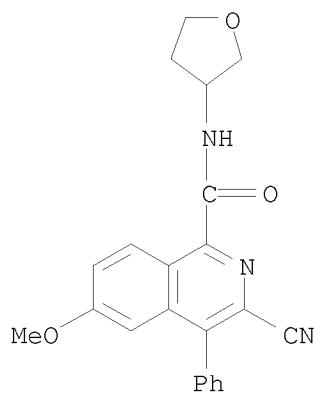
RN 849547-43-9 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[1-(5-isoxazolyl)ethyl]-6-methoxy-4-phenyl-
(CA INDEX NAME)

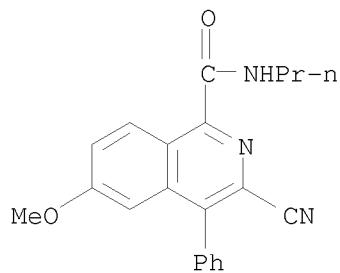
STN



RN 849547-45-1 HCAPLUS
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(tetrahydro-3-furanyl)- (CA INDEX NAME)



RN 849547-47-3 HCAPLUS
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-propyl- (CA INDEX NAME)

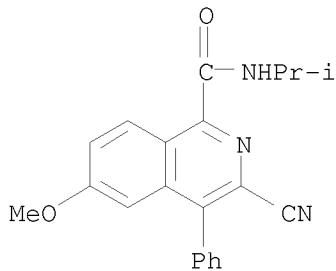


Updated Search

STN

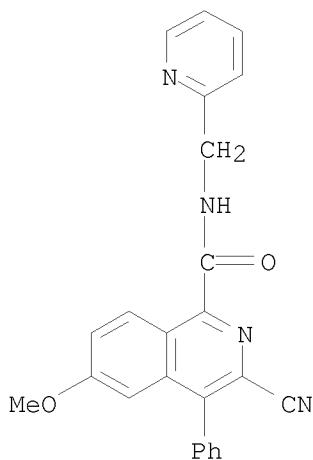
RN 849547-49-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(1-methylethyl)-4-phenyl-
(CA INDEX NAME)



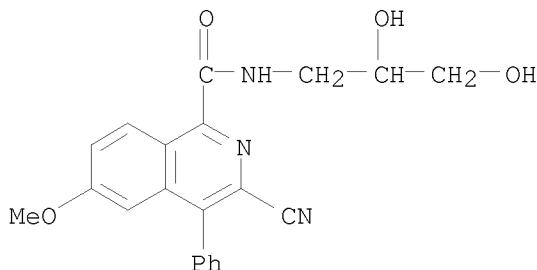
RN 849547-50-8 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(2-pyridinylmethyl)- (CA INDEX NAME)



RN 849547-51-9 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2,3-dihydroxypropyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

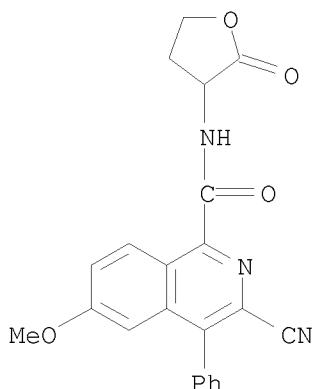


Updated Search

STN

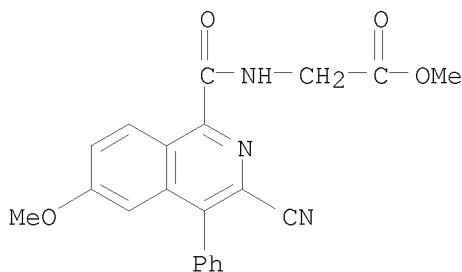
RN 849547-52-0 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(tetrahydro-2-oxo-3-furanyl)- (CA INDEX NAME)



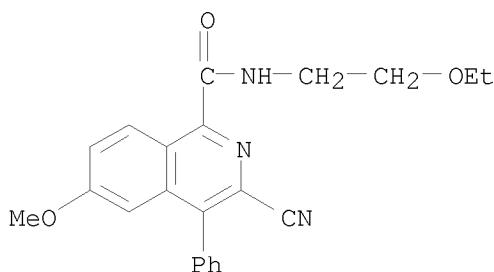
RN 849547-53-1 HCPLUS

CN Glycine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]-, methyl ester (CA INDEX NAME)



RN 849547-54-2 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-ethoxyethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

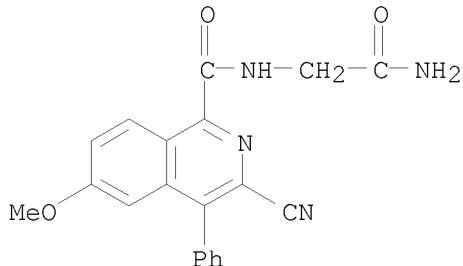


RN 849547-55-3 HCPLUS

Updated Search

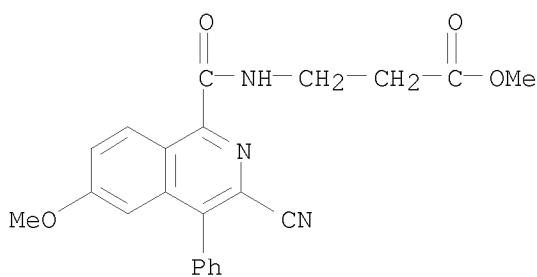
STN

CN 1-Isoquinolinecarboxamide, N-(2-amino-2-oxoethyl)-3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)



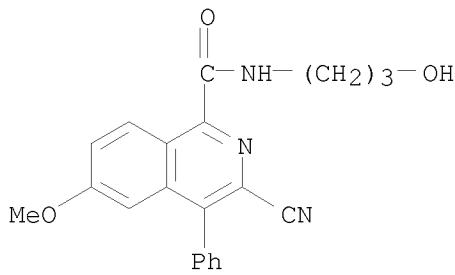
RN 849547-57-5 HCAPLUS

CN β-Alanine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]-, methyl ester (CA INDEX NAME)



RN 849547-59-7 HCAPLUS

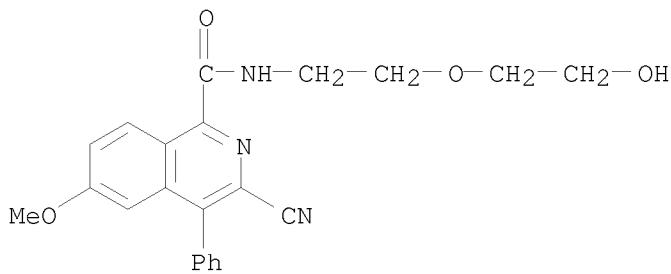
CN 1-Isoquinolinecarboxamide, 3-cyano-N-(3-hydroxypropyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-61-1 HCAPLUS

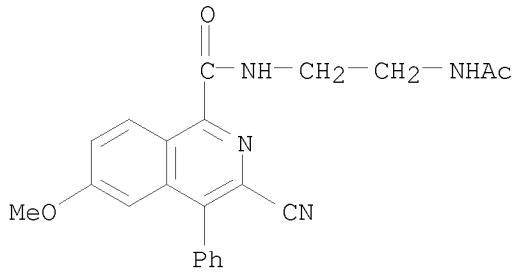
CN 1-Isoquinolinecarboxamide, 3-cyano-N-[2-(2-hydroxyethoxy)ethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

STN



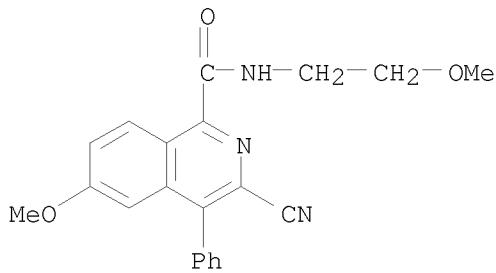
RN 849547-63-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, N-[2-(acetylamo)ethyl]-3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-65-5 HCAPLUS

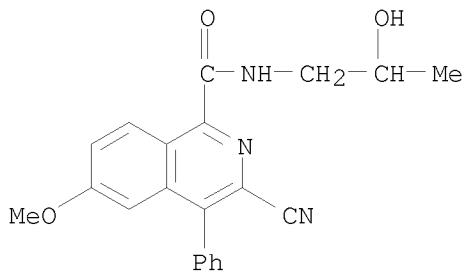
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-methoxyethyl)-4-phenyl- (CA INDEX NAME)



RN 849547-67-7 HCAPLUS

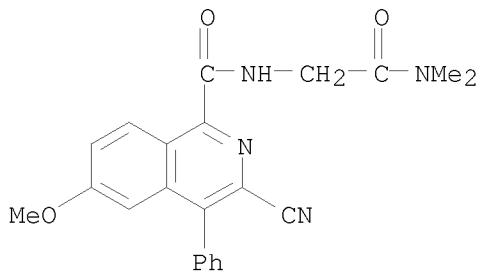
CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-hydroxypropyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

STN



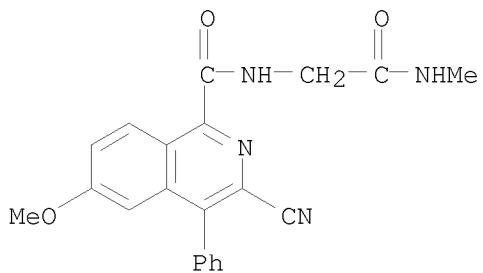
RN 849547-68-8 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[2-(dimethylamino)-2-oxoethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-69-9 HCPLUS

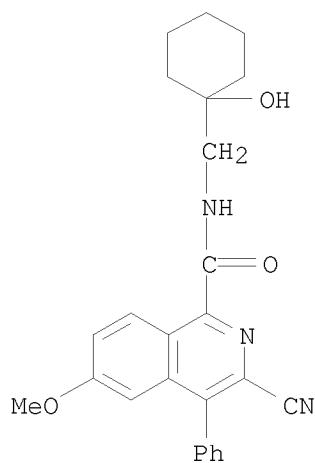
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-[2-(methylamino)-2-oxoethyl]-4-phenyl- (CA INDEX NAME)



RN 849547-71-3 HCPLUS

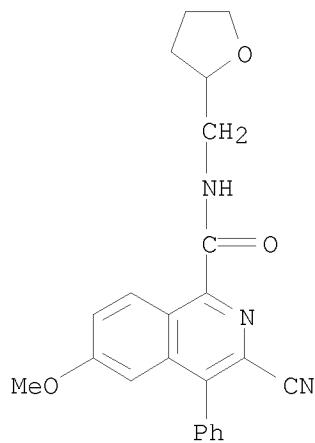
CN 1-Isoquinolinecarboxamide, 3-cyano-N-[(1-hydroxycyclohexyl)methyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

STN



RN 849547-73-5 HCPLUS

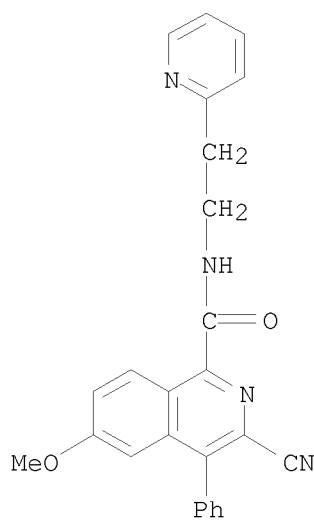
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[(tetrahydro-2-furanyl)methyl]- (CA INDEX NAME)



RN 849547-75-7 HCPLUS

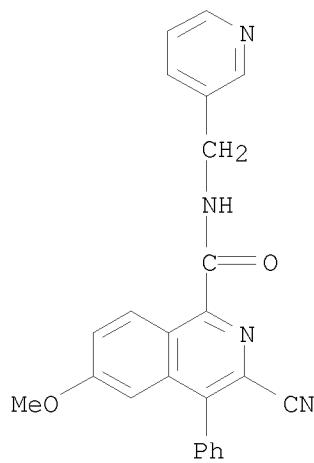
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[2-(2-pyridinyl)ethyl]- (CA INDEX NAME)

STN



RN 849547-76-8 HCAPLUS

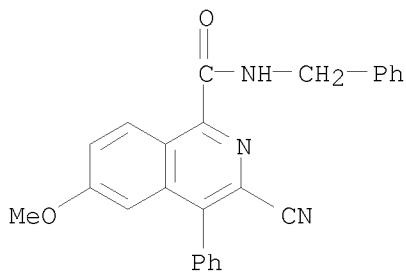
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(3-pyridinylmethyl)- (CA INDEX NAME)



RN 849547-78-0 HCAPLUS

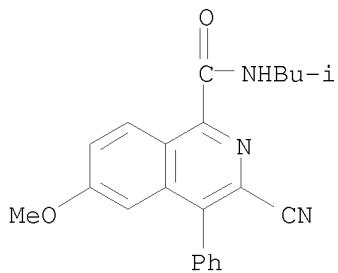
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(phenylmethyl)- (CA INDEX NAME)

STN



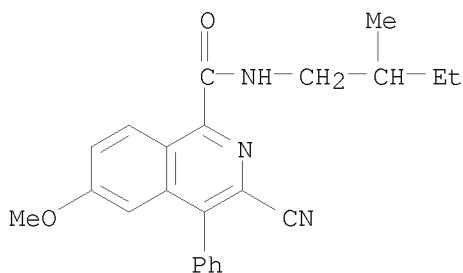
RN 849547-80-4 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-methylpropyl)-4-phenyl-
(CA INDEX NAME)



RN 849547-81-5 HCAPLUS

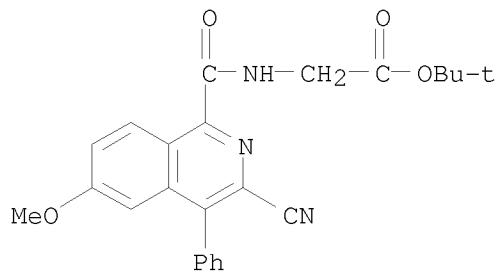
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-methylbutyl)-4-phenyl-
(CA INDEX NAME)



RN 849547-83-7 HCAPLUS

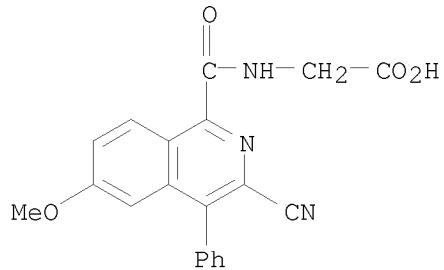
CN Glycine, N-[3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl]carbonyl]-,
1,1-dimethylethyl ester (CA INDEX NAME)

STN



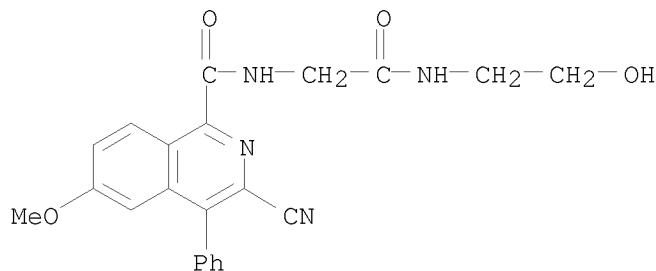
RN 849547-85-9 HCPLUS

CN Glycine, N-[3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl]carbonyl- (CA INDEX NAME)



RN 849547-87-1 HCPLUS

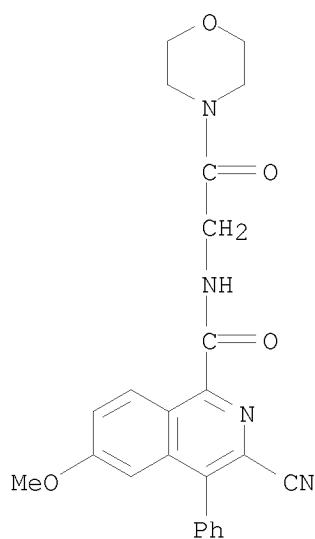
CN 1-Isoquinolinecarboxamide, 3-cyano-N-[2-[(2-hydroxyethyl)amino]-2-oxoethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)



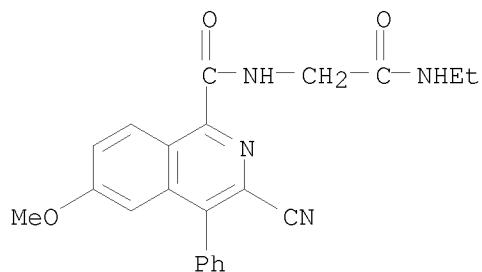
RN 849547-88-2 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-[2-(4-morpholinyl)-2-oxoethyl]-4-phenyl- (CA INDEX NAME)

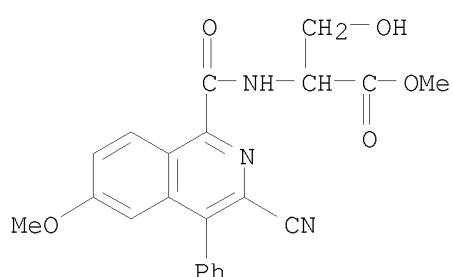
STN



RN 849547-90-6 HCAPLUS
CN 1-Isoquinolinecarboxamide, 3-cyano-N-[2-(ethylamino)-2-oxoethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-91-7 HCAPLUS
CN Serine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]-, methyl ester (CA INDEX NAME)

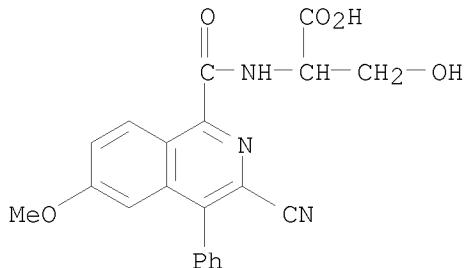


RN 849547-92-8 HCAPLUS

Updated Search

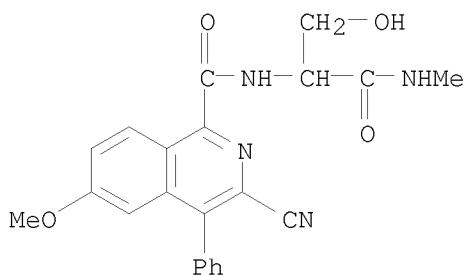
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CN Serine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]- (CA INDEX NAME)



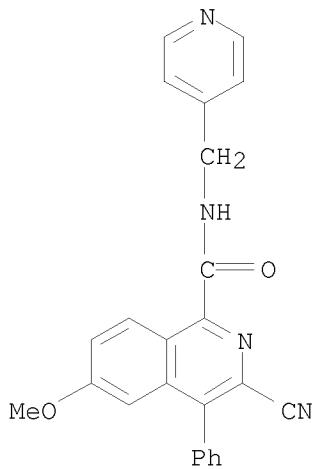
RN 849547-93-9 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[1-(hydroxymethyl)-2-(methylamino)-2-oxoethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-95-1 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(4-pyridinylmethyl)- (CA INDEX NAME)

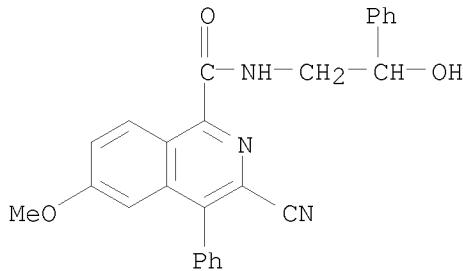


Updated Search

STN

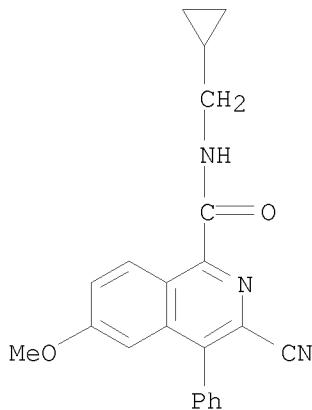
RN 849547-96-2 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-hydroxy-2-phenylethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-97-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(cyclopropylmethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

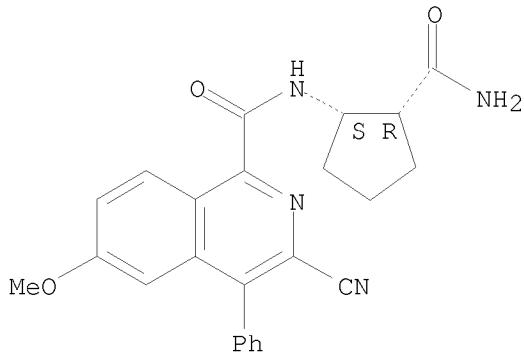


RN 849547-99-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, N-[(1S,2R)-2-(aminocarbonyl)cyclopentyl]-3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

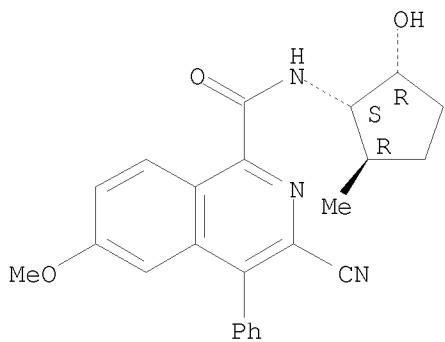
STN



RN 849548-00-1 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[(1S,2R,5R)-2-hydroxy-5-methylcyclopentyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

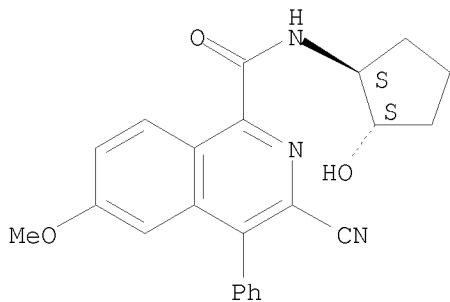
Absolute stereochemistry.



RN 849548-01-2 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[(1S,2S)-2-hydroxycyclopentyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 849548-02-3 HCAPLUS

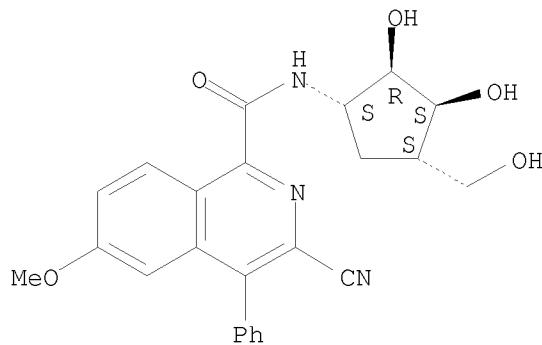
CN 1-Isoquinolinecarboxamide, 3-cyano-N-[(1S,2R,3S,4S)-2,3-dihydroxy-4-

Updated Search

STN

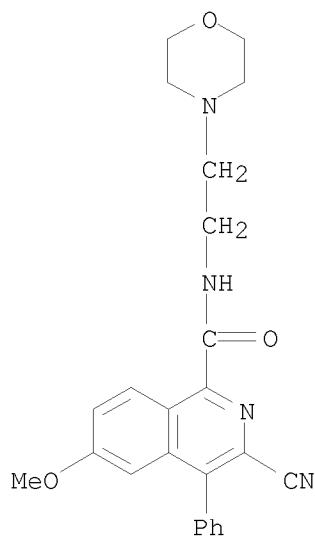
(hydroxymethyl)cyclopentyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 849548-03-4 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-[2-(4-morpholinyl)ethyl]-4-phenyl- (CA INDEX NAME)

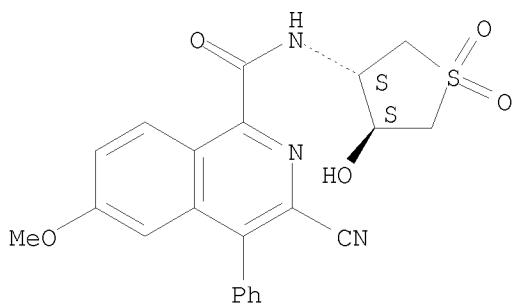


RN 849548-04-5 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[(3S,4S)-tetrahydro-4-hydroxy-1,1-dioxido-3-thienyl]- (CA INDEX NAME)

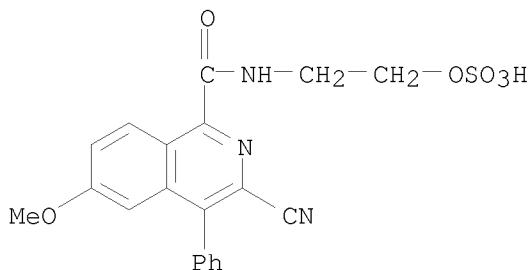
Absolute stereochemistry.

STN



RN 849548-05-6 HCAPLUS

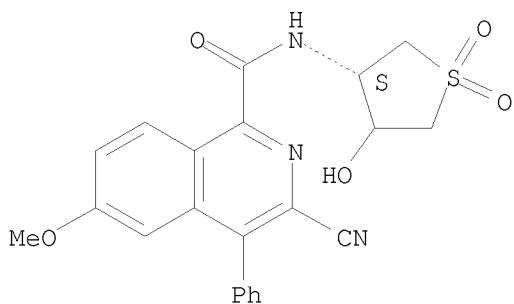
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[2-(sulfoxy)ethyl]- (CA INDEX NAME)



RN 849548-06-7 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[(3S)-tetrahydro-4-hydroxy-1,1-dioxido-3-thienyl]- (CA INDEX NAME)

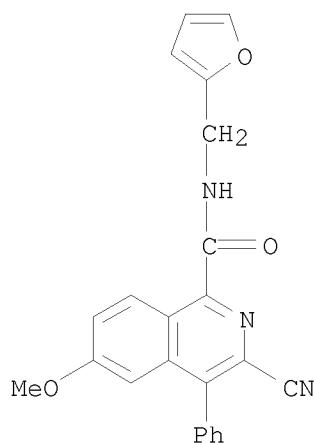
Absolute stereochemistry.



RN 849548-07-8 HCAPLUS

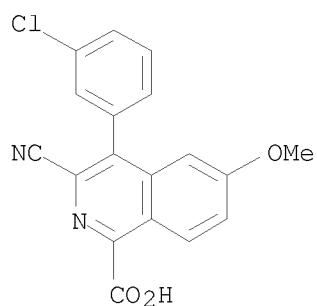
CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-furanyl methyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

STN



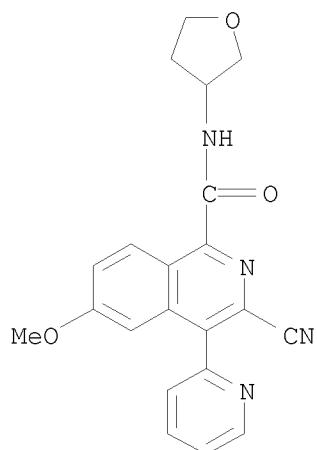
RN 849548-08-9 HCPLUS

CN 1-Isoquinolinecarboxylic acid, 4-(3-chlorophenyl)-3-cyano-6-methoxy- (CA INDEX NAME)



RN 849548-09-0 HCPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-(2-pyridinyl)-N-(tetrahydro-3-furanyl)- (CA INDEX NAME)

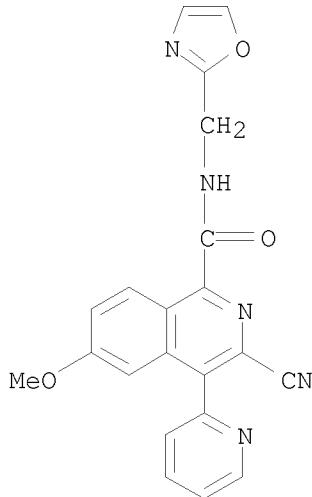


Updated Search

STN

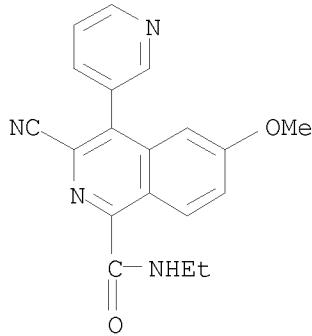
RN 849548-10-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-oxazolylmethyl)-4-(2-pyridinyl)- (CA INDEX NAME)



RN 849548-12-5 HCAPLUS

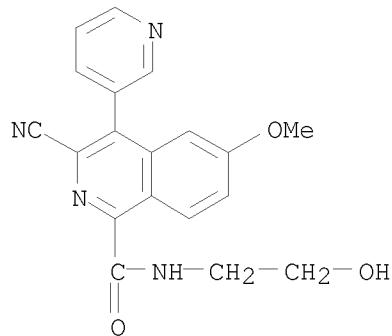
CN 1-Isoquinolinecarboxamide, 3-cyano-N-ethyl-6-methoxy-4-(3-pyridinyl)- (CA INDEX NAME)



RN 849548-14-7 HCAPLUS

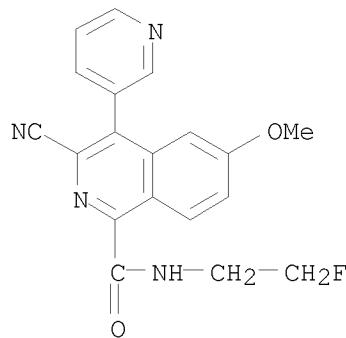
CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-hydroxyethyl)-6-methoxy-4-(3-pyridinyl)- (CA INDEX NAME)

STN



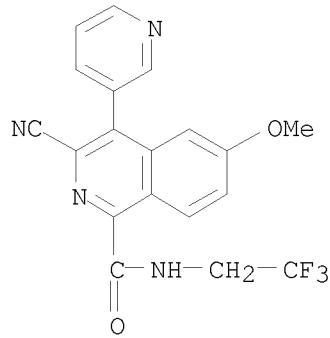
RN 849548-16-9 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-fluoroethyl)-6-methoxy-4-(3-pyridinyl)- (CA INDEX NAME)



RN 849548-18-1 HCAPLUS

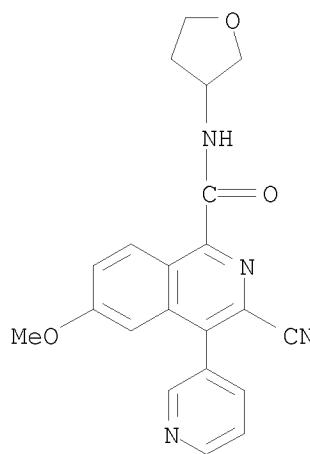
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-(3-pyridinyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



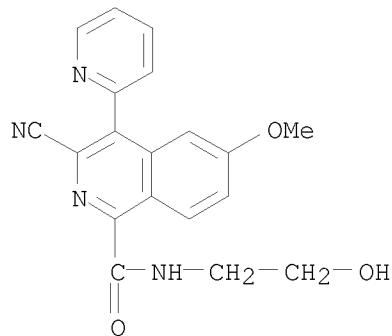
RN 849548-20-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-(3-pyridinyl)-N-(tetrahydro-3-furanyl)- (CA INDEX NAME)

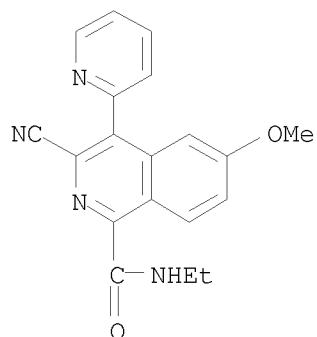
STN



RN 849548-22-7 HCAPLUS
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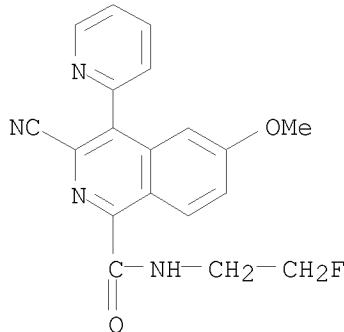
RN 849548-23-8 HCAPLUS
CN 1-Isoquinolinecarboxamide, 3-cyano-N-ethyl-6-methoxy-4-(2-pyridinyl)- (CA INDEX NAME)



STN

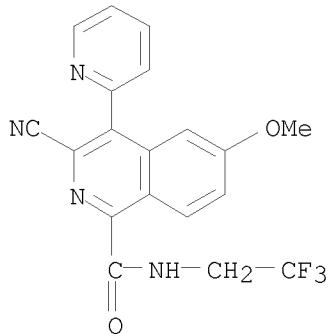
RN 849548-24-9 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-fluoroethyl)-6-methoxy-4-(2-pyridinyl)- (CA INDEX NAME)



RN 849548-25-0 HCAPLUS

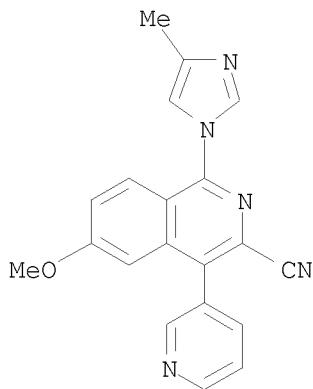
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-(2-pyridinyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



RN 849548-26-1 HCAPLUS

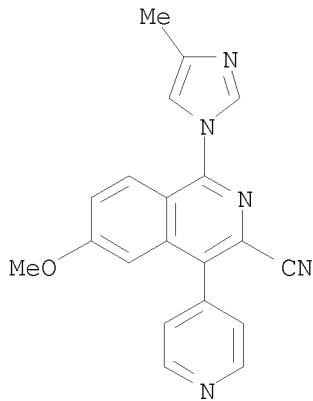
CN 3-Isoquinolinecarbonitrile, 6-methoxy-1-(4-methyl-1H-imidazol-1-yl)-4-(3-pyridinyl)- (CA INDEX NAME)

STN



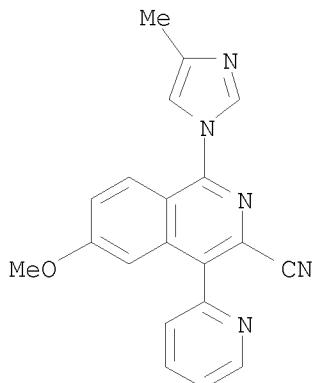
RN 849548-32-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-1-(4-methyl-1H-imidazol-1-yl)-4-(4-pyridinyl)- (CA INDEX NAME)



RN 849548-33-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-1-(4-methyl-1H-imidazol-1-yl)-4-(2-pyridinyl)- (CA INDEX NAME)

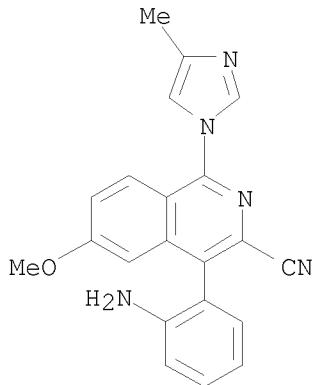


Updated Search

STN

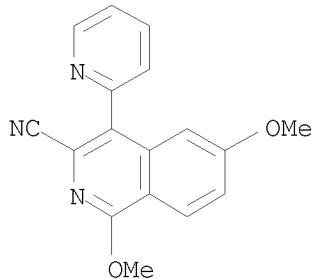
RN 849548-34-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(2-aminophenyl)-6-methoxy-1-(4-methyl-1H-imidazol-1-yl)- (CA INDEX NAME)



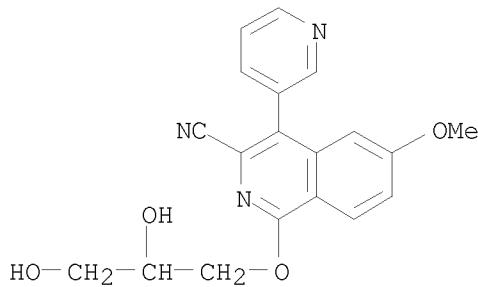
RN 849548-37-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1,6-dimethoxy-4-(2-pyridinyl)- (CA INDEX NAME)



RN 849548-38-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(2,3-dihydroxypropoxy)-6-methoxy-4-(3-pyridinyl)- (CA INDEX NAME)

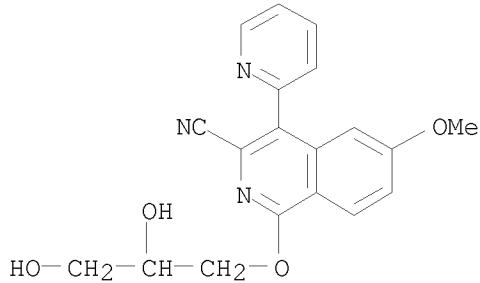


RN 849548-39-6 HCAPLUS

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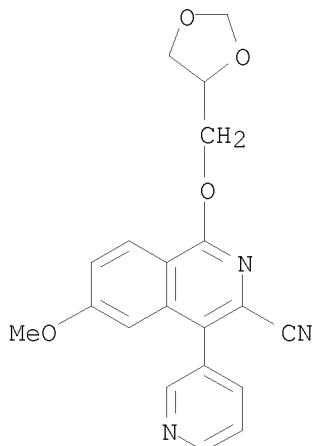
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CN 3-Isoquinolinecarbonitrile, 1-(2,3-dihydroxypropoxy)-6-methoxy-4-(2-pyridinyl)- (CA INDEX NAME)



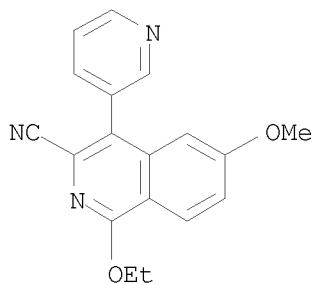
RN 849548-40-9 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-(1,3-dioxolan-4-ylmethoxy)-6-methoxy-4-(3-pyridinyl)- (CA INDEX NAME)



RN 849548-42-1 HCPLUS

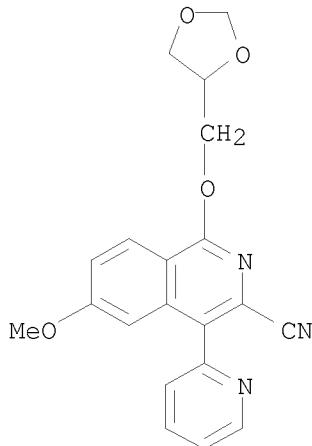
CN 3-Isoquinolinecarbonitrile, 1-ethoxy-6-methoxy-4-(3-pyridinyl)- (CA INDEX NAME)



STN

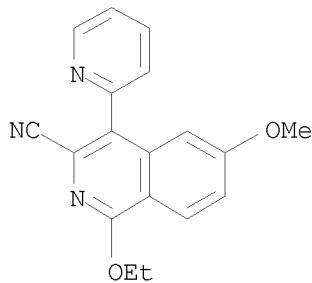
RN 849548-43-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(1,3-dioxolan-4-ylmethoxy)-6-methoxy-4-(2-pyridinyl)- (CA INDEX NAME)



RN 849548-44-3 HCAPLUS

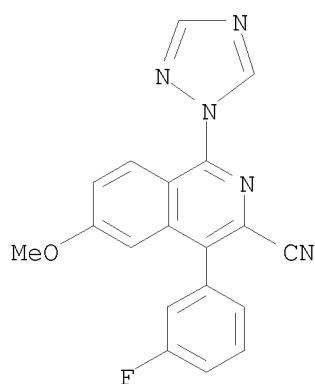
CN 3-Isoquinolinecarbonitrile, 1-ethoxy-6-methoxy-4-(2-pyridinyl)- (CA INDEX NAME)



RN 849548-46-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(1H-1,2,4-triazol-1-yl)- (CA INDEX NAME)

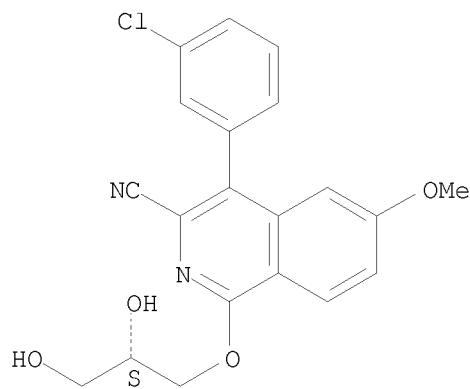
STN



RN 849548-47-6 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[(2S)-2,3-dihydroxypropoxy]-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

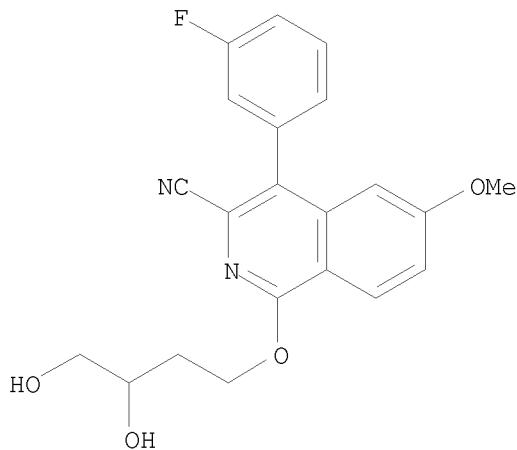


RN 849548-48-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(3,4-dihydroxybutoxy)-4-(3-fluorophenyl)-6-methoxy-, (+)- (CA INDEX NAME)

Rotation (+).

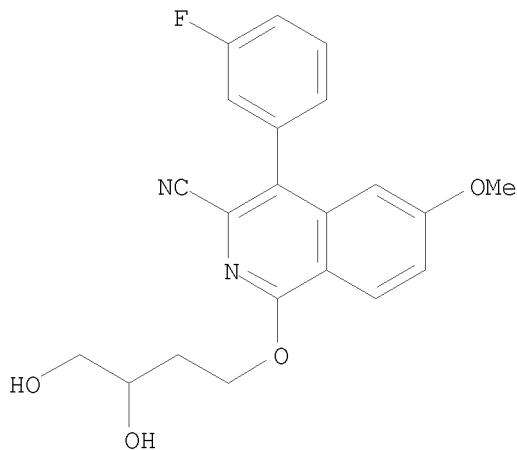
STN



RN 849548-49-8 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-(3,4-dihydroxybutoxy)-4-(3-fluorophenyl)-6-methoxy-, (-) - (CA INDEX NAME)

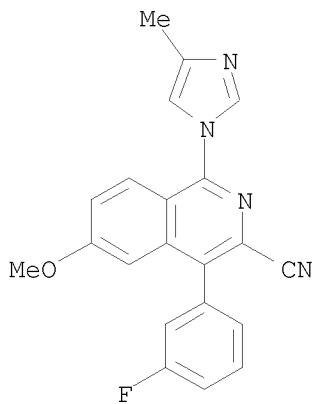
Rotation (-).



RN 849548-50-1 HCPLUS

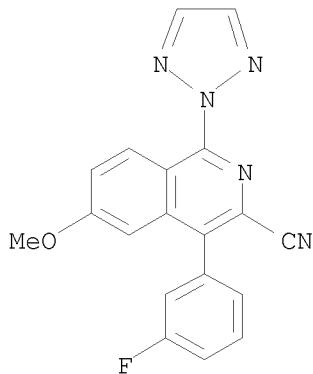
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(4-methyl-1H-imidazol-1-yl)- (CA INDEX NAME)

STN



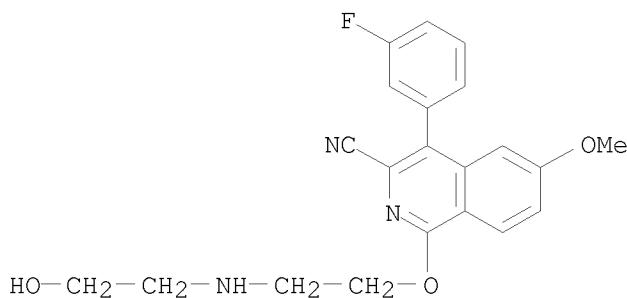
RN 849548-51-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(2H-1,2,3-triazol-2-yl)- (CA INDEX NAME)



RN 849548-52-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-[2-[(2-hydroxyethyl)amino]ethoxy]-6-methoxy- (CA INDEX NAME)

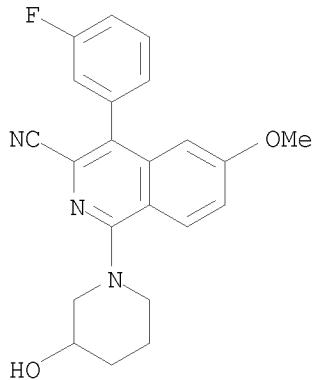


RN 849548-53-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-(3-hydroxy-1-piperidinyl)-6-methoxy- (CA INDEX NAME)

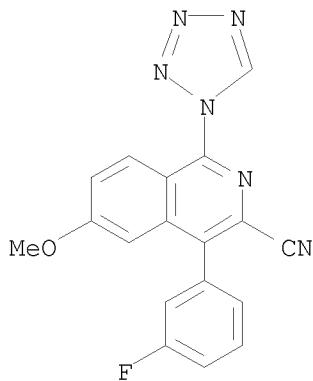
Updated Search

STN



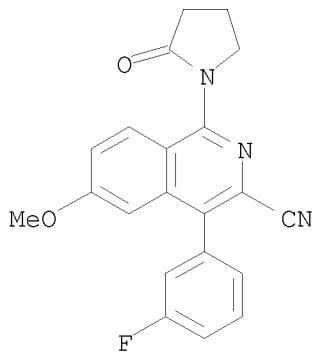
RN 849548-54-5 HCPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(1H-tetrazol-1-yl)- (CA INDEX NAME)



RN 849548-55-6 HCPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(2-oxo-1-pyrrolidinyl)- (CA INDEX NAME)

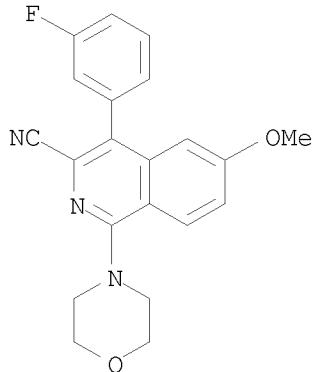


Updated Search

STN

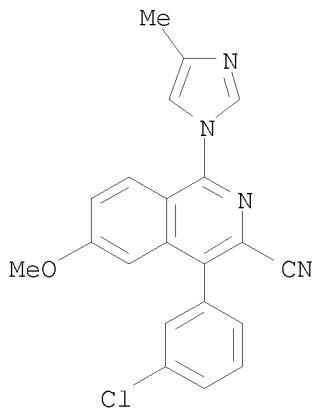
RN 849548-56-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(4-morpholinyl)-
(CA INDEX NAME)



RN 849548-57-8 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-(4-methyl-1H-imidazol-1-yl)- (CA INDEX NAME)

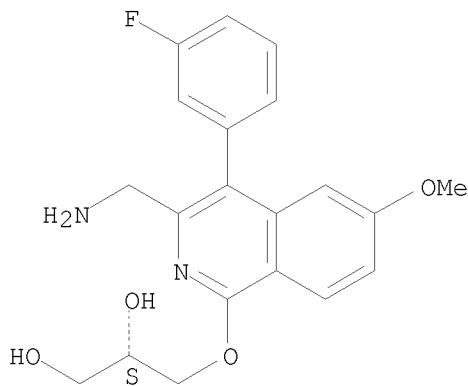


RN 849548-58-9 HCAPLUS

CN 1,2-Propanediol, 3-[{3-(aminomethyl)-4-(3-fluorophenyl)-6-methoxy-1-isoquinolinyl]oxy]-, (2S)- (CA INDEX NAME)

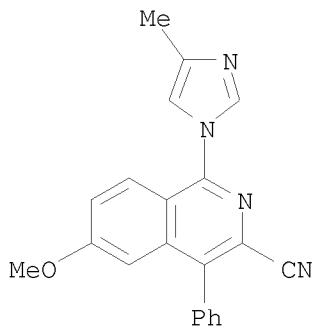
Absolute stereochemistry.

STN



RN 849548-59-0 HCAPLUS

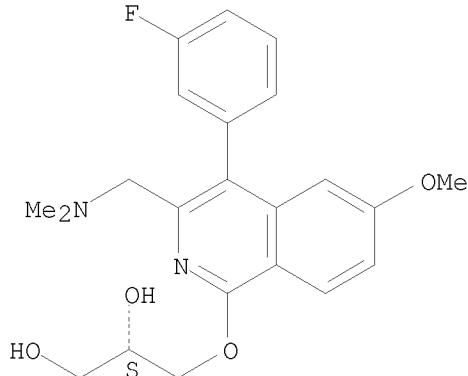
CN 3-Isoquinolinecarbonitrile, 6-methoxy-1-(4-methyl-1H-imidazol-1-yl)-4-phenyl- (CA INDEX NAME)



RN 849548-60-3 HCAPLUS

CN 1,2-Propanediol, 3-[(3-[(dimethylamino)methyl]-4-(3-fluorophenyl)-6-methoxy-1-isoquinolinyl]oxy]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

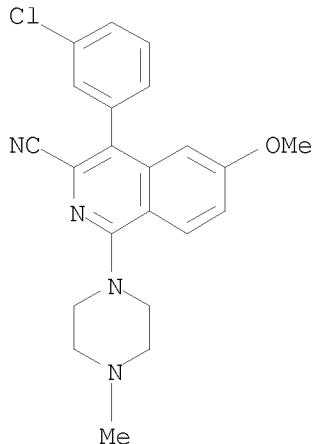


Updated Search

STN

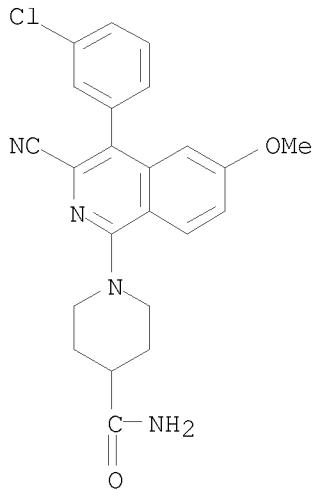
RN 849548-61-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-(4-methyl-1-piperazinyl)- (CA INDEX NAME)



RN 849548-64-7 HCAPLUS

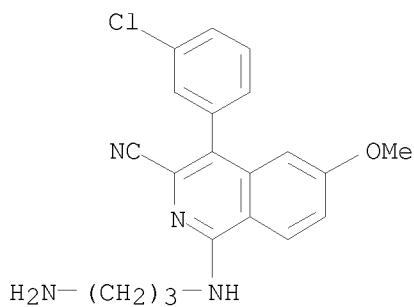
CN 4-Piperidinecarboxamide, 1-[4-(3-chlorophenyl)-3-cyano-6-methoxy-1-isoquinolinyl]- (CA INDEX NAME)



RN 849548-65-8 HCAPLUS

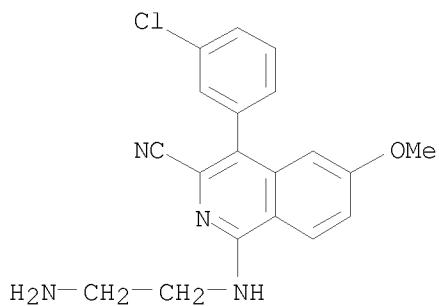
CN 3-Isoquinolinecarbonitrile, 1-[(3-aminopropyl)amino]-4-(3-chlorophenyl)-6-methoxy- (CA INDEX NAME)

STN



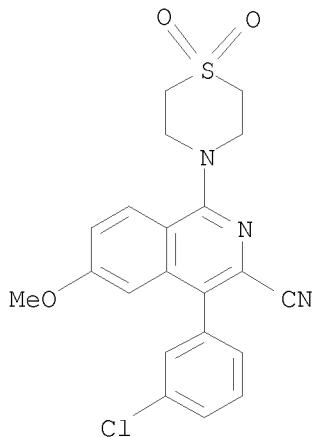
RN 849548-66-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2-aminoethyl)amino]-4-(3-chlorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849548-67-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-(1,1-dioxido-4-thiomorpholinyl)-6-methoxy- (CA INDEX NAME)

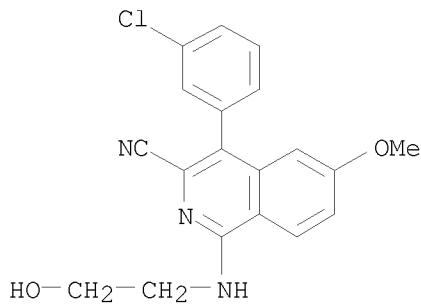


RN 849548-68-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[(2-hydroxyethyl)amino]-6-methoxy- (CA INDEX NAME)

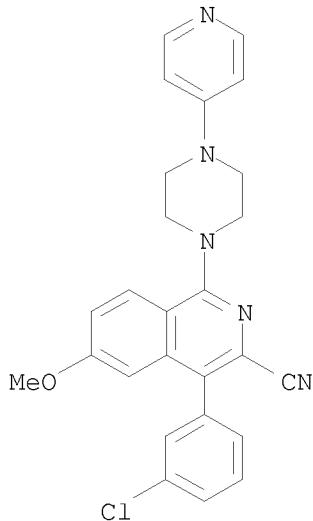
Updated Search

STN



RN 849548-70-5 HCAPLUS

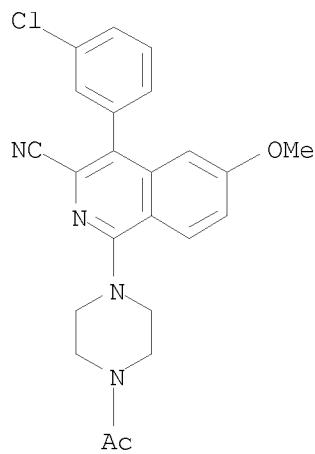
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-[4-(4-pyridinyl)-1-piperazinyl]- (CA INDEX NAME)



RN 849548-71-6 HCAPLUS

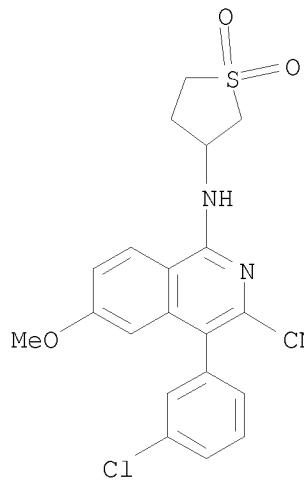
CN 3-Isoquinolinecarbonitrile, 1-(4-acetyl-1-piperazinyl)-4-(3-chlorophenyl)-6-methoxy- (CA INDEX NAME)

STN



RN 849548-72-7 HCAPLUS

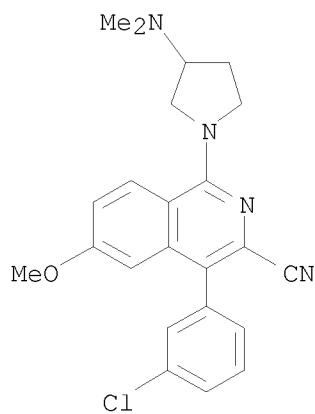
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-[(tetrahydro-1,1-dioxido-3-thienyl)amino]- (CA INDEX NAME)



RN 849548-73-8 HCAPLUS

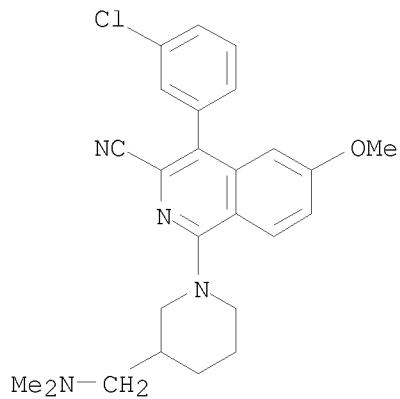
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[3-(dimethylamino)-1-pyrrolidinyl]-6-methoxy- (CA INDEX NAME)

STN



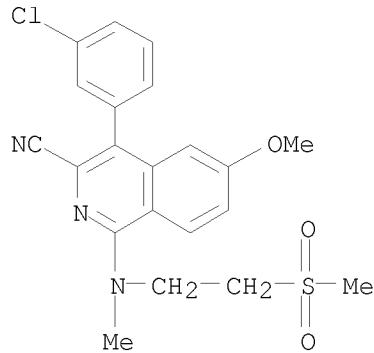
RN 849548-74-9 HCPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[3-[(dimethylamino)methyl]-1-piperidinyl]-6-methoxy- (CA INDEX NAME)



RN 849548-75-0 HCPLUS

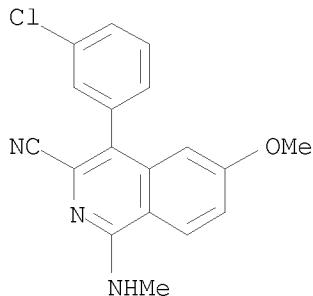
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-[methyl[2-(methylsulfonyl)ethyl]amino]- (CA INDEX NAME)



STN

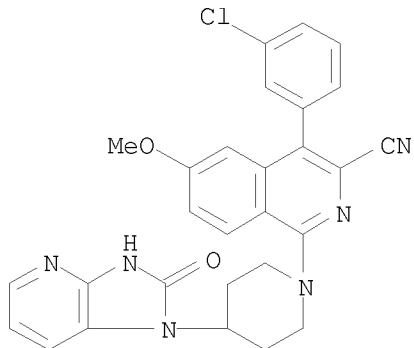
RN 849548-76-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-(methylamino)-
(CA INDEX NAME)



RN 849548-77-2 HCAPLUS

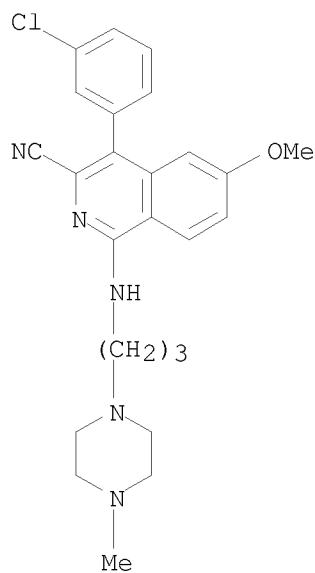
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[4-(2,3-dihydro-2-oxo-1H-imidazo[4,5-b]pyridin-1-yl)-1-piperidinyl]-6-methoxy- (CA INDEX NAME)



RN 849548-79-4 HCAPLUS

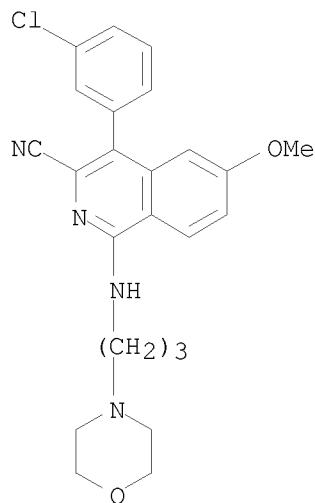
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-[3-(4-methyl-1-piperazinyl)propyl]amino- (CA INDEX NAME)

STN



RN 849548-80-7 HCAPLUS

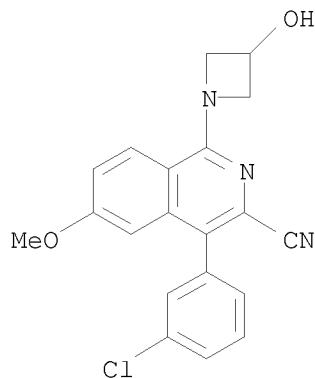
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-[3-(4-morpholinyl)propyl]amino- (CA INDEX NAME)



RN 849548-81-8 HCAPLUS

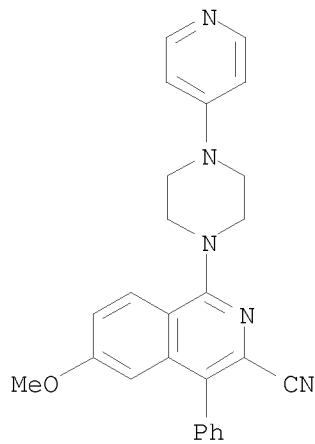
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-(3-hydroxy-1-azetidinyl)-6-methoxy- (CA INDEX NAME)

STN



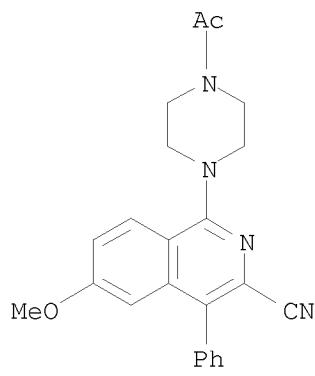
RN 849548-83-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-[4-(4-pyridinyl)-1-piperazinyl]- (CA INDEX NAME)



RN 849548-84-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(4-acetyl-1-piperazinyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

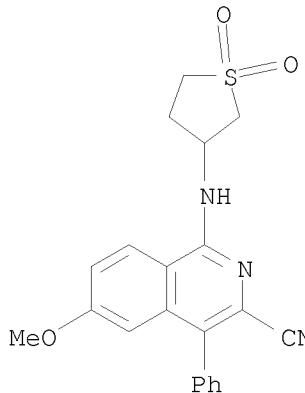


Updated Search

STN

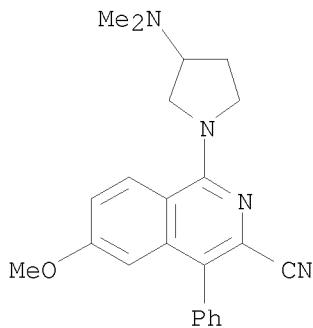
RN 849548-85-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-[(tetrahydro-1,1-dioxido-3-thienyl)amino]- (CA INDEX NAME)



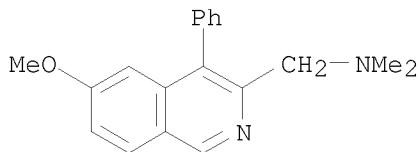
RN 849548-86-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[3-(dimethylamino)-1-pyrrolidinyl]-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849549-04-8 HCAPLUS

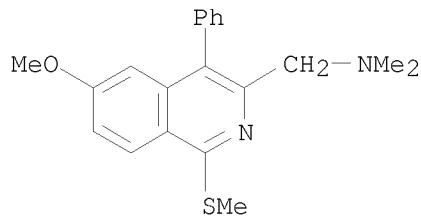
CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-4-phenyl- (CA INDEX NAME)



RN 849549-05-9 HCAPLUS

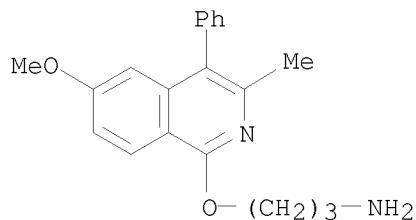
CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-1-(methylthio)-4-phenyl- (CA INDEX NAME)

STN



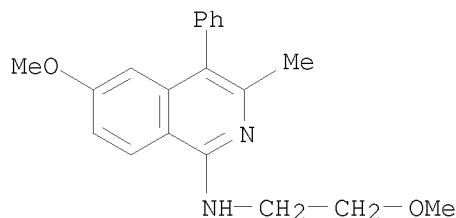
RN 849549-06-0 HCPLUS

CN 1-Propanamine, 3-[(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)oxy]- (CA INDEX NAME)



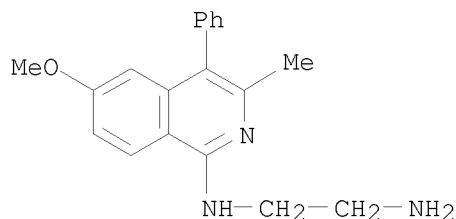
RN 849549-07-1 HCPLUS

CN 1-Isoquinolinamine, 6-methoxy-N-(2-methoxyethyl)-3-methyl-4-phenyl- (CA INDEX NAME)



RN 849549-08-2 HCPLUS

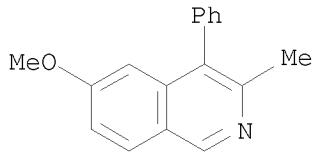
CN 1,2-Ethanediamine, N1-(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)- (CA INDEX NAME)



STN

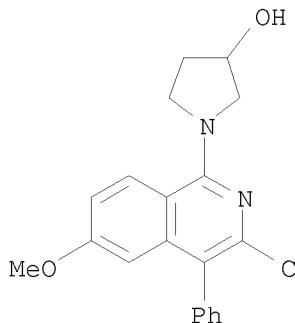
RN 849549-09-3 HCAPLUS

CN Isoquinoline, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



RN 849549-10-6 HCAPLUS

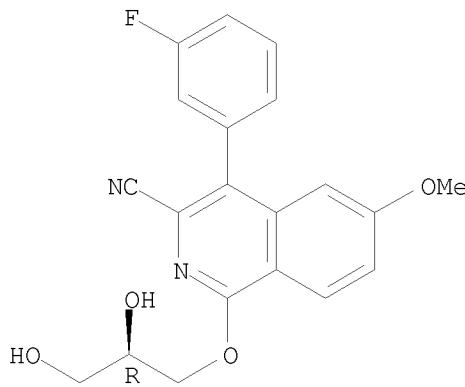
CN 3-Isoquinolinecarbonitrile, 1-(3-hydroxy-1-pyrrolidinyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849549-11-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2R)-2,3-dihydroxypropoxy]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.



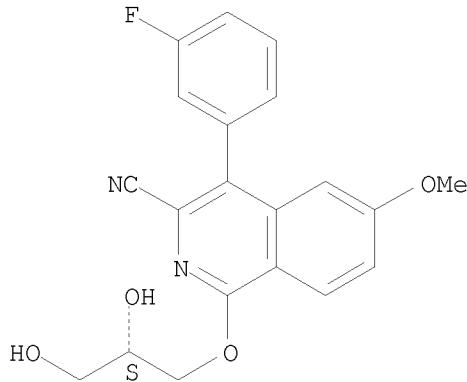
RN 849549-12-8 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-2,3-dihydroxypropoxy]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Updated Search

STN

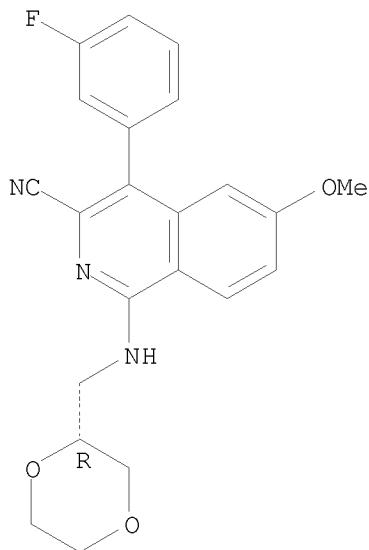
Absolute stereochemistry.



RN 849549-13-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2R)-1,4-dioxan-2-ylmethyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

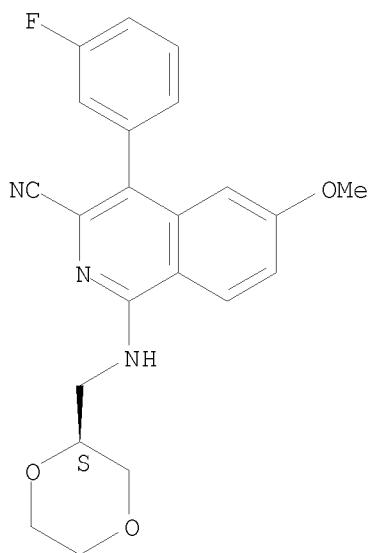


RN 849549-14-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-1,4-dioxan-2-ylmethyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

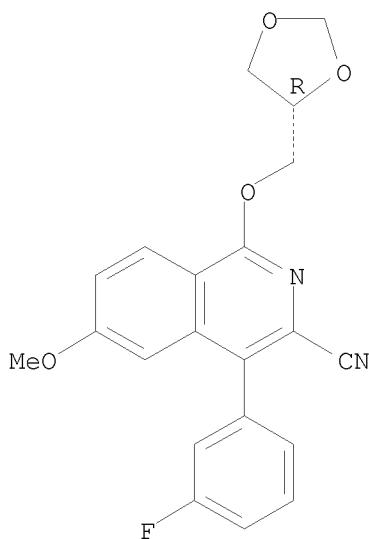
STN



RN 849549-15-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(4R)-1,3-dioxolan-4-ylmethoxy]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

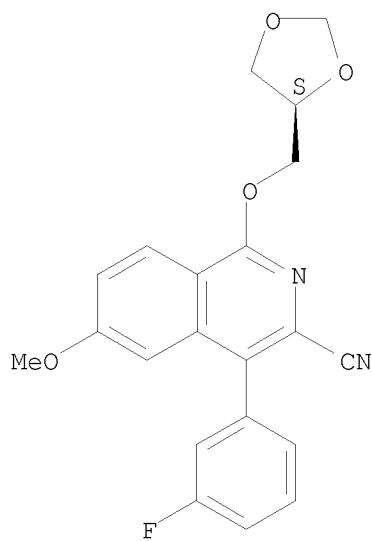


RN 849549-16-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(4S)-1,3-dioxolan-4-ylmethoxy]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

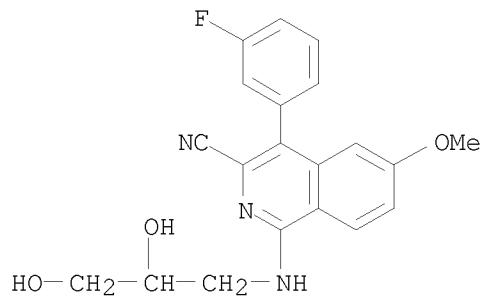
Absolute stereochemistry.

STN



RN 849549-17-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2,3-dihydroxypropyl)amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

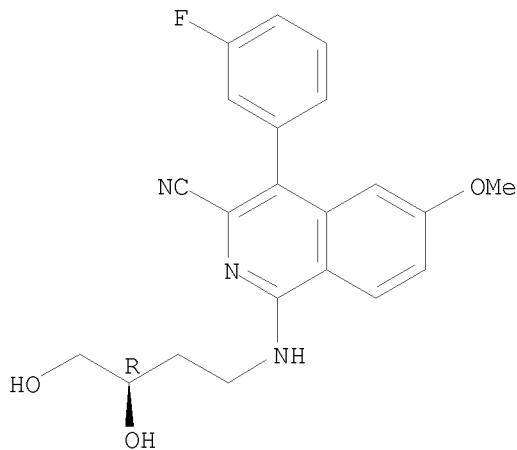


RN 849549-18-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3R)-3,4-dihydroxybutyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

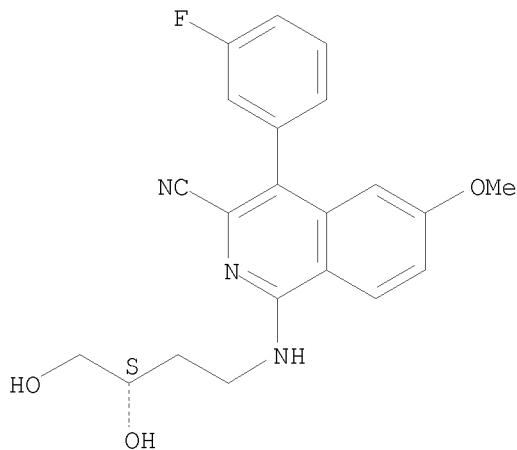
STN



RN 849549-19-5 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3S)-3,4-dihydroxybutyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

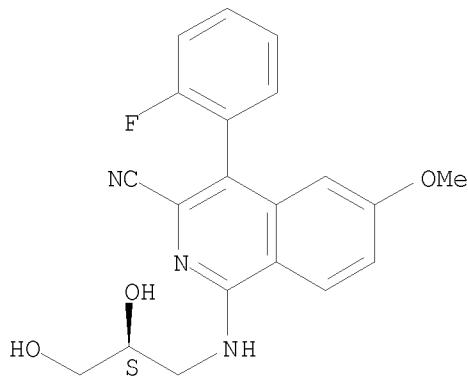


RN 849549-20-8 HCPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-2,3-dihydroxypropyl]amino]-4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

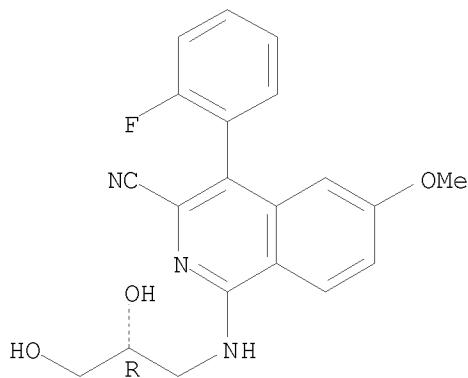
STN



RN 849549-21-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2R)-2,3-dihydroxypropyl]amino]-4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)

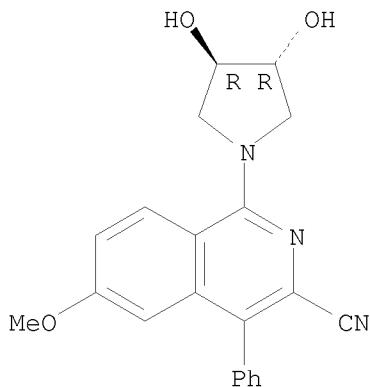
Absolute stereochemistry.



RN 849549-25-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3R,4R)-3,4-dihydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl-, rel- (CA INDEX NAME)

Relative stereochemistry.

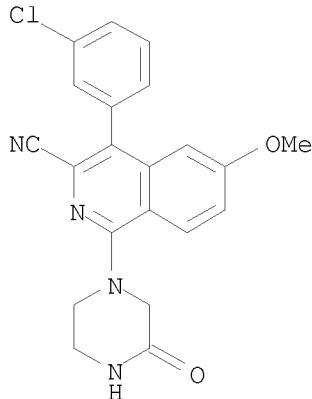


Updated Search

STN

RN 849549-32-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-(3-oxo-1-piperazinyl)- (CA INDEX NAME)



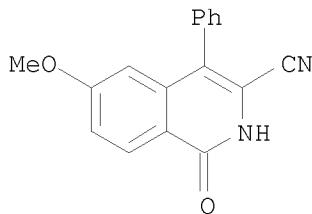
IT 849549-26-4 849549-27-5 849549-29-7

849549-31-1 849635-33-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of isoquinoline derivs. as potassium channel inhibitors)

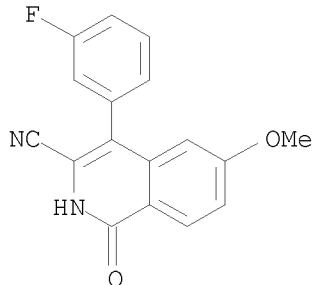
RN 849549-26-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1,2-dihydro-6-methoxy-1-oxo-4-phenyl- (CA INDEX NAME)



RN 849549-27-5 HCAPLUS

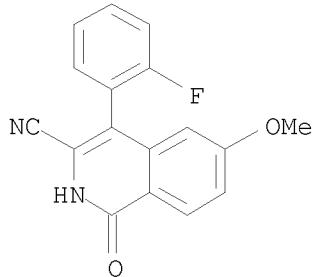
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1,2-dihydro-6-methoxy-1-oxo- (CA INDEX NAME)



STN

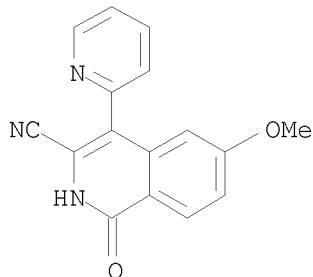
RN 849549-29-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(2-fluorophenyl)-1,2-dihydro-6-methoxy-1-oxo-
(CA INDEX NAME)



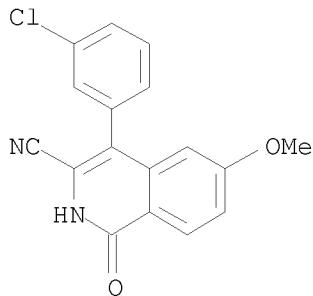
RN 849549-31-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1,2-dihydro-6-methoxy-1-oxo-4-(2-pyridinyl)-
(CA INDEX NAME)



RN 849635-33-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1,2-dihydro-6-methoxy-1-oxo-
(CA INDEX NAME)



IT 849424-95-9P 849548-87-4P 849548-88-5P

849548-89-6P 849548-90-9P 849548-91-0P

849548-93-2P 849548-94-3P 849548-99-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

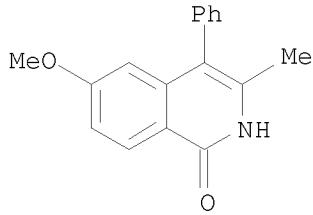
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(Reactant or reagent)

(preparation of isoquinoline derivs. as potassium channel inhibitors)

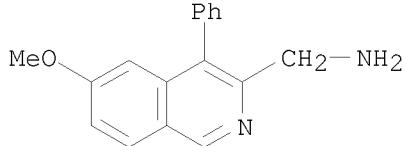
RN 849424-95-9 HCPLUS

CN 1(2H)-Isoquinolinone, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



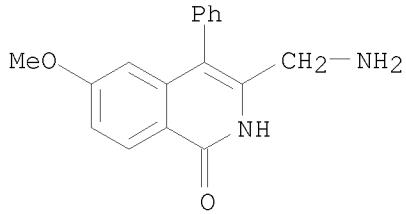
RN 849548-87-4 HCPLUS

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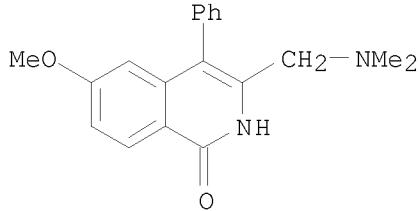
RN 849548-88-5 HCPLUS

CN 1(2H)-Isoquinolinone, 3-(aminomethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849548-89-6 HCPLUS

CN 1(2H)-Isoquinolinone, 3-[dimethylamino)methyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

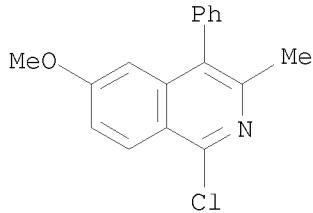


Updated Search

STN

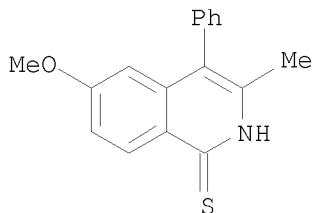
RN 849548-90-9 HCAPLUS

CN Isoquinoline, 1-chloro-6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



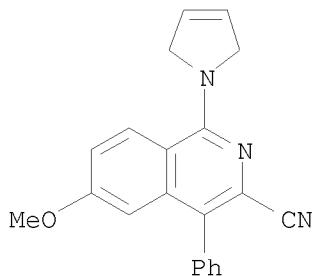
RN 849548-91-0 HCAPLUS

CN 1(2H)-Isoquinolinethione, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



RN 849548-93-2 HCAPLUS

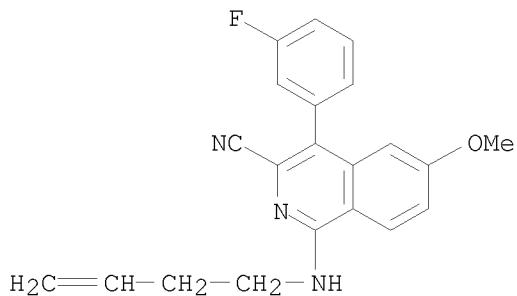
CN 3-Isoquinolinecarbonitrile, 1-(2,5-dihydro-1H-pyrrol-1-yl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849548-94-3 HCAPLUS

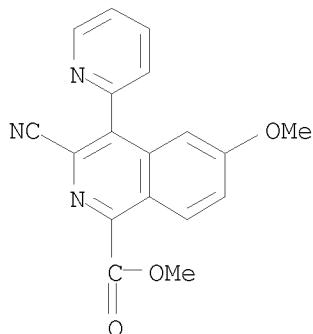
CN 3-Isoquinolinecarbonitrile, 1-(3-buten-1-ylamino)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

STN



RN 849548-99-8 HCPLUS

CN 1-Isoquinolinecarboxylic acid, 3-cyano-6-methoxy-4-(2-pyridinyl)-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 19:20:54 ON 05 NOV 2009)

FILE 'REGISTRY' ENTERED AT 19:21:02 ON 05 NOV 2009

L1 STRUCTURE uploaded
L2 759 S 1L
L3 1677 S L1 FULL

FILE 'HCPLUS' ENTERED AT 19:24:12 ON 05 NOV 2009

L4 376 S L3
L5 58 S L3/USES
L6 4 S L4 AND TROTTER, B?/AU

=> s l4 not l6

L7 372 L4 NOT L6

=> s l7 and nanda, k?/au
311 NANDA, K?/AU

Updated Search

STN

L8 0 L7 AND NANDA, K?/AU

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9 KETT, N?/AU

L9 0 L7 AND KETT, N?/AU

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122 DINSMORE, C?/AU

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=> s 17 and ponticello, g?/au
111 PONTICELLO, G?/AU
L11 0 L7 AND PONTICELLO, G?/AU

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175 CLAREMON, D?/AU
L12 0 L7 AND CLAREMON, D?/AU

=> s 14 and pd < october 2003
23911169 PD < OCTOBER 2003
(PD<20031000)

L13 310 L4 AND PD < OCTOBER 2003

=> s 15 and pd < october 2003
23911169 PD < OCTOBER 2003
(PD<20031000)

L14 29 L5 AND PD < OCTOBER 2003

=> d 114, ibib abs fhitstr, 1-29
THE ESTIMATED COST FOR THIS REQUEST IS 163.56 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L14 ANSWER 1 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:497495 HCPLUS
DOCUMENT NUMBER: 143:43783
TITLE: Preparation of (guanidinophenyl)isoquinolines and
related compounds as MC4-R agonists
INVENTOR(S): Boyce, Rustum; Chu, Daniel
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S.
Ser. No. 351,574.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

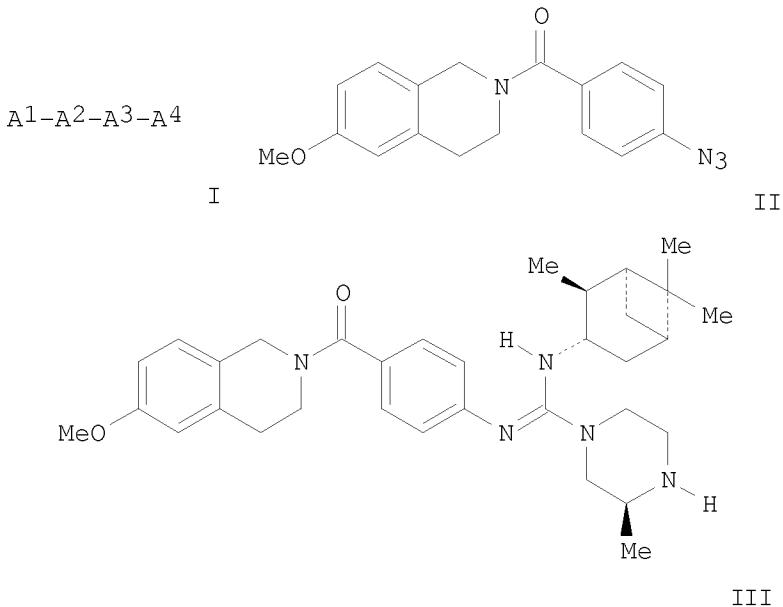
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050124652	A1	20050609	US 2005-503392	20050126
US 20030195187	A1	20031016	US 2003-351574	20030127
WO 2003066597	A2	20030814	WO 2003-US1078	20030203 <--
WO 2003066597	A3	20040401		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-353188P P 20020204
US 2003-351574 A2 20030127
WO 2003-US1078 W 20030203

OTHER SOURCE(S): CASREACT 143:43783; MARPAT 143:43783

GI



AB Title compds. I [A1 = NR4C(=NR3)NR1R2, N=C(NR3R4)(NR1R2); R1 = H, (un)substituted alkyl, alkenyl, etc.; R2 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R3 = (un)substituted aryl, alkyl, alkenyl, etc.; R4 = H, (un)substituted alkyl, alkenyl, etc.; A2 = (un)substituted aryl, heteroaryl; A3 = covalent bond, linking group, e.g., O, S, CO, etc.; A4 = (un)substituted arylalkyl, heteroarylalkyl, aryl, etc.] and their pharmaceutically acceptable salts were prepared. For example, trimethylphosphine mediated reduction of phenylazide II followed by the sequential addition of (1S,2S,3S,5S)-2,6,6-trimethylbicyclo[3.1.1]heptan-3-isocyanate and (S)-(+)-2-methylpiperazine, afforded (guanidinophenyl)isoquinoline III. Compds. I are claimed to be useful for the treatment of obesity and type II diabetes.

IT 581101-76-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

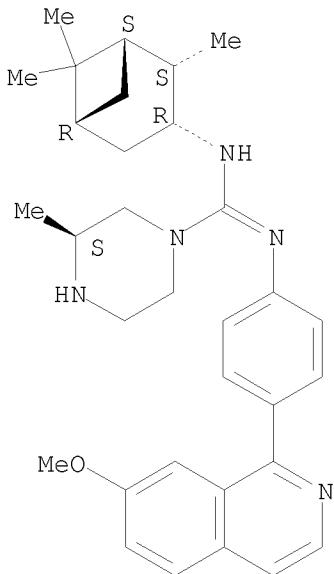
STN

(preparation of (guanidinophenyl)isoquinolines and related compds. as MC4-R agonists)

RN 581101-76-0 HCPLUS

CN 1-Piperazinecarboximidamide, N-[4-(7-methoxy-1-isoquinolinyl)phenyl]-3-methyl-N'-(1S,2S,3R,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl]-, (3S)-(CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 2 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:941009 HCPLUS

DOCUMENT NUMBER: 140:280814

TITLE: Effects of topoisomerases inhibitors protoberberine on Leishmania donovani growth, macrophage function, and infection

AUTHOR(S): Marquis, Jean-Francois; Makhey, Darshan; LaVoie, Edmond J.; Olivier, Martin

CORPORATE SOURCE: Departement de Biologie Medicale, Faculte de Medecine, Centre de Recherche en Infectiologie du CHUQ, Universite Laval, Sainte-Foy, QC, G1V 4G2, Can.

SOURCE: Journal of Parasitology (2003), 89(5), 1048-1052

CODEN: JOPAA2; ISSN: 0022-3395

PUBLISHER: American Society of Parasitologists

DOCUMENT TYPE: Journal

LANGUAGE: English

AB DNA topoisomerases play a pivotal role in the regulation of cell division. Inhibition of Leishmania spp. topoisomerases represents an alternative to control parasite growth. Cancer research led to the development of several potent topoisomerase inhibitors such as topoisomerase 1, topoisomerase 17, or both (monobenzimidazole, terbenzimidazole, and protoberberine alkaloid-related compds.) that are effective antitumor agents. In the present study, we evaluated the efficacy of these compds.

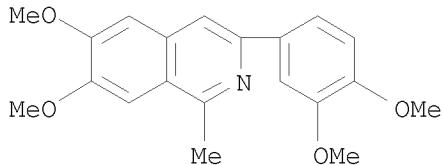
against Leishmania spp. growth in vitro. Some protoberberine compds. showed pronounced antileishmanial activity and were selected for further anal. in macrophages. These compds. did not affect macrophage viability and only slightly reduced macrophage nitric oxide generation in response to interferon- γ . Moreover, exposure of infected macrophages to these compds. significantly reduced parasite loads. Collectively, our data suggest that protoberberine-related compds. have powerful antileishmania action and that minor structural variations among them can substantially improve their activity to restrict Leishmania spp. infection in vitro.

IT 35989-93-6

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(topoisomerase inhibitors protoberberine derivs. effects on Leishmania donovani growth, macrophage function, and infection)

RN 35989-93-6 HCPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:633668 HCPLUS

DOCUMENT NUMBER: 139:197505

TITLE: Preparation of aryl- or heteroaryl-containing guanidines as melanocortin-4-receptor agonists useful against disorders such as obesity or type II diabetes

INVENTOR(S): Boyce, Rustum; Chu, Daniel

PATENT ASSIGNEE(S): Chiron Corporation, USA

SOURCE: PCT Int. Appl., 102 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

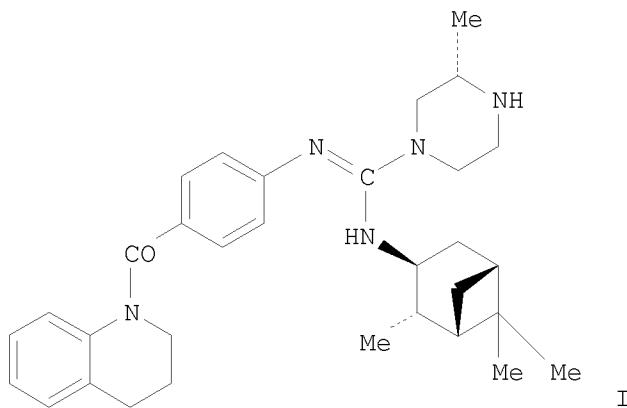
PATENT INFORMATION:

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WO 2003066597	A2	20030814	WO 2003-US1078	20030203 <--
WO 2003066597	A3	20040401		
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PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 US 20030195187 A1 20031016 US 2003-351574 20030127
 AU 2003216053 A1 20030902 AU 2003-216053 20030203 <--
 EP 1478626 A2 20041124 EP 2003-737536 20030203
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 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
 JP 2006503799 T 20060202 JP 2003-565971 20030203
 US 20050124652 A1 20050609 US 2005-503392 20050126
 PRIORITY APPLN. INFO.: US 2002-353188P P 20020204
 US 2003-351574 A 20030127
 WO 2003-US1078 W 20030203

OTHER SOURCE(S): MARPAT 139:197505

GI



AB A variety of small, guanidino group-containing mols. (I; A1-A2-A3-A4; variables defined below; e.g. (3S)-N'-(4-(3,4-dihydroquinolin-1(2H)-ylcarbonyl)phenyl)-3-methyl-N-[(1S,2S,3S,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl]piperazine-1-carboximidamide (shown as I)) capable of acting as MC4-R agonists are provided. The compds. are useful in treating MC4-R mediated diseases and may be formulated into pharmaceutical formulations and compns. Although the methods of preparation are not claimed, several example preps. of I and a number of example preps. of intermediates are included; 131 addnl. examples of I are tabulated with mass spectral characterization data. Some of the I have -log EC50 values above .apprx.3. Compds. I showed beneficial effects in in vivo studies on energy intake, body weight, hyperinsulinemia, and glucose levels in male 9-10 wk old ob/ob mice that display early onset of obesity, insulin resistance and diabetes due to leptin deficiency. For I: A1 = R1'R2'NC(:NR3')NR4'-, R1'R2'NC(NR3'R4'):N-; R1' = H, and (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, heterocyclyl, arylalkyl, heteroarylalkyl, and cycloalkylalkyl; R2' = (un)substituted alkyl,

alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, heterocyclyl, arylalkyl, heteroarylalkyl, and cycloalkylalkyl; or R1' and R2', together with the N to which they are bound, form a (un)substituted heterocyclyl or heteroaryl; R3' = (un)substituted aryl, alkyl, alkenyl, alkynyl, cycloalkyl, heteroaryl, heterocyclyl, heterocyclylalkyl, arylalkyl, heteroarylalkyl, and cycloalkylalkyl; R4' = H, and (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, heterocyclylalkyl, cycloalkylalkyl, aryl, heteroaryl, heterocyclyl, arylalkyl, and heteroarylalkyl. A2 = (un)substituted aryl and heteroaryl; A3 is a covalent bond such that A2 is directly bonded to A4, or A3 is a linking group O, S, -NRa-, -C(O)-, -C(O)O-, -NRaC(O)-, -SO2NRa-, -C(S)-, -C(O)S-, -P(O)Rb-, -SO2-, and -S(O)-, wherein if A3 is a linking group, then it is bonded to A2 and A4 in a configuration A2-O-A4, A2-S-A4, A2-NRa-A4, A2-C(O)-A4, A2-C(O)O-A4, A4-C(O)O-A2, A2-NRaC(O)-A4, A4-NRaC(O)-A2, A2-SO2NRa-A4, A4-SO2NRa-A2, A2-C(S)-A4, A2-(C:O)S-A4, A4-(C:O)S-A2, A2-(P:O)Rb-A4, A2-SO2-A4, and A2-S(O)-A4 provided that if A3 is a linking group with the configuration A4-NRaC(O)-A2, then A2 is not a (un)substituted Ph and is not a (un)substituted 6-membered N-containing heteroaryl. A4 = (un)substituted arylalkyl, heteroarylalkyl, aryl, heteroaryl, heterocyclyl, cycloalkyl, heterocyclylalkyl, cycloalkylalkyl, alkenyl, alkynyl, and alkyl; Ra = H, and (un)substituted arylalkyl, heteroarylalkyl, aryl, heteroaryl, heterocyclyl, cycloalkyl, heterocyclylalkyl, cycloalkylalkyl, alkenyl, alkynyl, and alkyl; Rb = (un)substituted arylalkyl, heteroarylalkyl, aryl, heteroaryl, heterocyclyl, cycloalkyl, heterocyclylalkyl, cycloalkylalkyl, alkenyl, alkynyl, and alkyl.

IT 581101-76-0P, (3S)-3-Methyl-N-[4-[7-(methyloxy)isoquinolin-1-yl]phenyl]-N'-(1S,2S,3R,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl)piperazine-1-carboximidamide

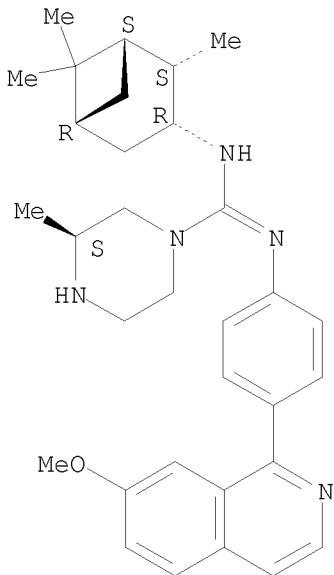
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of aryl- or heteroaryl-containing guanidines as melanocortin-4-receptor agonists useful against disorders such as obesity or type II diabetes)

RN 581101-76-0 HCPLUS

CN 1-Piperazinecarboximidamide, N-[4-(7-methoxy-1-isoquinolinyl)phenyl]-3-methyl-N'-(1S,2S,3R,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl-, (3S)-(CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
 (5 CITINGS)
 REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

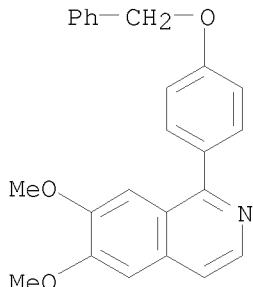
L14 ANSWER 4 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:311225 HCPLUS
 DOCUMENT NUMBER: 139:270245
 TITLE: Structure-based approach to falcipain-2 inhibitors:
 synthesis and biological evaluation of
 1,6,7-Trisubstituted dihydroisoquinolines and
 isoquinolines
 AUTHOR(S): Batra, Sanjay; Sabnis, Yogesh A.; Rosenthal, Philip
 J.; Avery, Mitchell A.
 CORPORATE SOURCE: Medicinal Chemistry Division, Central Drug Research
 Institute, Lucknow, 226001, India
 SOURCE: Bioorganic & Medicinal Chemistry (2003),
 11(10), 2293-2299
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:270245
 AB 1,4,7-Trisubstituted isoquinolines were designed, synthesized and
 evaluated for their inhibition against *Plasmodium falciparum* cysteine
 protease falcipain-2. The 1-benzylxyphenyl-dihydroisoquinoline and
 -isoquinoline derivs. were found to exhibit better activity against
 falcipain-2 than their corresponding 1-hydroxyphenyl or 1-methoxyphenyl
 analogs. The docking scores correlate with the IC50 values of compds. and
 give a high coefficient correlation of 0.94.
 IT 605657-60-1P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
 preparation); THU (Therapeutic use); BIOL (Biological study); USES
 (Uses); RACT (Reactant or reagent); USES (Uses)

STN

(synthesis, antimalarial effect and structure-activity relationship of dihydroisoquinoline and isoquinoline derivs. as falcipain-2 inhibitors)

RN 605657-60-1 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-[4-(phenylmethoxy)phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 27 THERE ARE 27 CAPLUS RECORDS THAT CITE THIS RECORD (27 CITINGS)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:282400 HCPLUS
DOCUMENT NUMBER: 138:309280
TITLE: Combinations containing a phosphodiesterase inhibitor
INVENTOR(S): Cohen, David Saul
PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis-Erfindungen
Verwaltungsgesellschaft M.B.H.; Novartis Pharma GmbH
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003028730	A2	20030410	WO 2002-EP10826	20020926 <--
WO 2003028730	A3	20030904		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR				
US 20030114469	A1	20030619	US 2002-231427	20020828 <--
US 20030139429	A1	20030724	US 2002-236651	20020906 <--
US 7019010	B2	20060328		
CA 2458343	A1	20030410	CA 2002-2458343	20020926 <--
AU 2002338806	A1	20030414	AU 2002-338806	20020926 <--
EP 1432423	A2	20040630	EP 2002-777227	20020926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				

BR 2002012852	A	20041013	BR 2002-12852	20020926
JP 2005504113	T	20050210	JP 2003-532062	20020926
CN 1694707	A	20051109	CN 2002-819046	20020926
US 20060106039	A1	20060518	US 2006-324999	20060103
PRIORITY APPLN. INFO.:			US 2001-325485P	P 20010927
			US 2002-231427	B2 20020828
			US 2002-236651	A3 20020906
			WO 2002-EP10826	W 20020926

OTHER SOURCE(S): MARPAT 138:309280

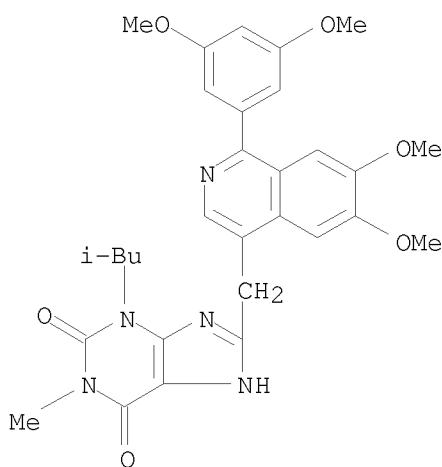
AB The present invention relates to a pharmaceutical composition, comprising (a) a phosphodiesterase 5 inhibitor or a pharmaceutically acceptable salt thereof and (b) at least one of the active ingredients selected from the group consisting of (i) an anti-diabetic agent; (ii) HMG-Co-A reductase inhibitors; (iii) an antihypertensive agent; and (iv) a serotonin reuptake inhibitor (SSRI) or, in each case, or a pharmaceutically acceptable salt thereof and a pharmaceutically acceptable carrier. The pharmaceutical composition may be employed for the treatment of sexual dysfunction, hyperglycemia, hyperinsulinemia, hyperlipidemia, hypertriglyceridemia, diabetes, insulin resistance, impaired glucose metabolism, conditions of impaired glucose tolerance (IGT), conditions of impaired fasting plasma glucose, obesity, diabetic retinopathy, diabetic nephropathy, glomerulosclerosis, diabetic neuropathy, syndrome X, erectile dysfunction, coronary heart disease, hypertension, especially ISH, angina pectoris, myocardial infarction, stroke, vascular restenosis, endothelial dysfunction, impaired vascular compliance, congestive heart failure.

IT 366444-39-5

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. containing PDE5 inhibitor in combination with antidiabetic, HMG-Co-A reductase inhibitor, antihypertensive, or serotonin reuptake inhibitor)

RN 366444-39-5 HCPLUS

CN 1H-Purine-2,6-dione, 8-[[1-(3,5-dimethoxyphenyl)-6,7-dimethoxy-4-isoquinolinyl]methyl]-3,9-dihydro-1-methyl-3-(2-methylpropyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(16 CITINGS)

STN

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 6 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:905931 HCAPLUS
DOCUMENT NUMBER: 137:389204
TITLE: Compositions for promoting healing of bone fracture containing phosphodiesterase 4 inhibitors
INVENTOR(S): Sakurai, Naoki; Takagi, Toshiki; Yanaka, Noriyuki; Horikiri, Yuji; Tamura, Takashi
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002094321	A1	20021128	WO 2002-JP4931	20020522 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2447619	A1	20021128	CA 2002-2447619	20020522 <--
AU 2002308878	A1	20021203	AU 2002-308878	20020522 <--
EP 1389468	A1	20040218	EP 2002-771772	20020522
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1520313	A	20040811	CN 2002-812733	20020522
MX 2003010679	A	20040302	MX 2003-10679	20031121
US 20040146561	A1	20040729	US 2003-478709	20031124
US 20080031958	A1	20080207	US 2007-826921	20070719
PRIORITY APPLN. INFO.:			JP 2001-154064	A 20010523
			WO 2002-JP4931	W 20020522
			US 2003-478709	A3 20031124

AB Disclosed are compns. for promoting healing of bone fracture which contain as the active ingredient a phosphodiesterase (PDE) 4 inhibitor having an effect of inhibiting PDE4, e.g. 2,3-bis(hydroxymethyl)-6,7-diethoxy-1-[1-(2-methoxyethyl)-2-oxo-4-pyridyl]-naphthalene and 2,3-bis(hydroxymethyl)-6,7-diethoxy-1-[2-(4-(3-pyridyl)-1(2H)-phthalazinone-2-yl)-4-pyridyl]-naphthalene, etc.. In particular, medicinal compns. containing the PDE4 inhibitor and a biocompatible and biodegradable polymer which exert an excellent effect of promoting quick healing of bone fracture when processed into dosage forms adequate for topical administration to bone fracture sites, for example, microspherical preps. These compns. are useful in treating bone fracture in, for example, aged persons, patients with diabetics and patients with osteoporosis which can be hardly repaired.

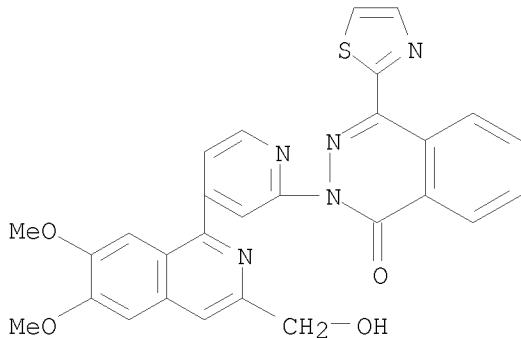
IT 209261-43-8

STN

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(compns. for promoting healing of bone fracture containing
phosphodiesterase 4 inhibitors)

RN 209261-43-8 HCPLUS

CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-
isoquinolinyl]-2-pyridinyl]-4-(2-thiazolyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:905929 HCPLUS

DOCUMENT NUMBER: 137:389203

TITLE: Therapeutic compositions for repairing chondropathy
containing phosphodiesterase 4 inhibitors

INVENTOR(S): Takigawa, Masaharu; Sakurai, Naoki; Takagi, Toshiki;
Yanaka, Noriyuki; Horikiri, Yuji; Tamura, Takashi

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 66 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002094320	A1	20021128	WO 2002-JP4930	20020522 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2447618	A1	20021128	CA 2002-2447618	20020522 <--

STN

AU 2002308877	A1 20021203	AU 2002-308877	20020522 <--
EP 1389467	A1 20040218	EP 2002-771771	20020522
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
CN 1537018	A 20041013	CN 2002-812647	20020522
MX 2003010672	A 20040302	MX 2003-10672	20031121
US 20040180900	A1 20040916	US 2003-478432	20031121
US 20070155652	A1 20070705	US 2007-707008	20070216
PRIORITY APPLN. INFO.:		JP 2001-154048	A 20010523
		WO 2002-JP4930	W 20020522
		US 2003-478432	A3 20031121

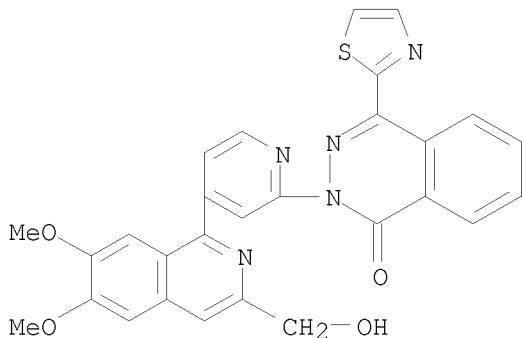
AB Therapeutic compns. for repairing chondropathy which contain as the active ingredient a phosphodiesterase (PDE) 4 inhibitor having an effect of inhibiting PDE4, e.g. 2,3-bis(hydroxymethyl)-6,7-diethoxy-1-[1-(2-methoxyethyl)-2-oxo-4-pyridyl]-naphthalene and 2,3-bis(hydroxymethyl)-6,7-diethoxy-1-[2-(4-(3-pyridyl)-1(2H)-phthalazinone-2-yl)-4-pyridyl]-naphthalene, etc. In particular, medicinal compns. containing the PDE4 inhibitor and a biocompatible and biodegradable polymer which exert an excellent effect of repairing cartilage when processed into dosage forms adequate for topical administration to sites suffering from chondropathy, for example, microspherical preps.

IT 209261-43-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic compns. for repairing chondropathy containing phosphodiesterase 4 inhibitors)

RN 209261-43-8 HCPLUS

CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-isoquinolinyl]-2-pyridinyl]-4-(2-thiazolyl)- (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 8 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:902258 HCPLUS

DOCUMENT NUMBER: 137:379992

TITLE: Method of inhibiting neoplastic cells with isoquinolinonecarboxylates

INVENTOR(S): Pamukcu, Rifat; Piazza, Gary A.

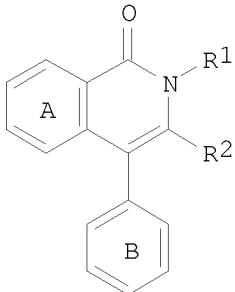
PATENT ASSIGNEE(S): Cell Pathways, Inc., USA

SOURCE: U.S., 119 pp.

STN

CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6486155	B1	20021126	US 1998-198413	19981124 <--
PRIORITY APPLN. INFO.:			US 1998-198413	19981124
OTHER SOURCE(S): GI	MARPAT	137:379992		



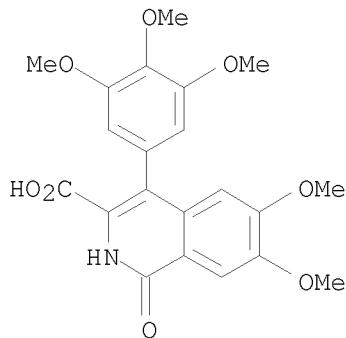
AB A method is claimed for inhibiting neoplasia (no data), particularly cancerous and precancerous lesions, by exposing the affected cells to 1-isoquinoline-3-carboxylates. Such compds. are effective in modulating apoptosis and eliminating and inhibiting the growth of neoplasias such as precancerous lesions, but are not characterized by the severe side reactions of conventional non-steroidal antiinflammatory drugs or other chemotherapeutics. Although the methods of preparation are not claimed, example preps. of 429 isoquinolines and 107 intermediates are included; these examples are referenced to PCT application WO 98/38168. Although the claims indicate I (ring A and ring B are the same or different and each a (un)substituted benzene ring, R1 is morpholine, R2 is -COOR3, and R3 is alkyl; e.g. 7-benzylxy-6-methoxy-3-methoxycarbonyl-2-morpholino-4-(3,4,5-trimethoxyphenyl)-1(2H)-isoquinolinone) or pharmaceutically acceptable salt thereof, the examples include a much broader variety of 1-isoquinoline-3-carboxylates.

IT 212489-07-1P, 3-Isoquinolinecarboxylic acid,
1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); USES (Uses)
(preparation of isoquinolinonecarboxylates for inhibiting neoplastic cells)

RN 212489-07-1 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)

STN



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 171 THERE ARE 171 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 9 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:624439 HCAPLUS

DOCUMENT NUMBER: 137:129831

TITLE: Method of extracting octaverine from Chinese herbal
medicine Poncirus trifoliata

INVENTOR(S): Hou, Tuanzhang

PATENT ASSIGNEE(S): Peop. Rep. China

SOURCE: Faming Zhuanli Shengqing Gongkai Shuomingshu, 3 pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent

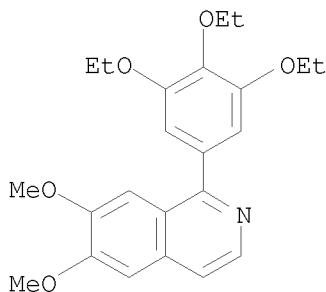
LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1318538	A	20011024	CN 2001-106994	20010411 <--
PRIORITY APPLN. INFO.:			CN 2001-106994	20010411
AB The method comprises extracting Poncirus trifoliata with water, concentrating, precipitating				
with alc., concentrating, filtering with sand, purifying on cation exchange resin				
column with NH4OH as eluent, concentrating, crystallizing, and recrystg.				
IT 549-68-8, Octaverine	RL: NPO (Natural product occurrence); PEP (Physical, engineering or chemical process); PYP (Physical process); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PROC (Process); USES (Uses) (extracting octaverine from Chinese herbal medicine)			
RN 549-68-8 HCAPLUS				
CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-trimethoxyphenyl)-	(CA INDEX NAME)			

STN



L14 ANSWER 10 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:293613 HCPLUS

DOCUMENT NUMBER: 136:309858

TITLE: Preparation of isoquinolines, isochromanones and isothiochromanones as inhibitors of tumor necrosis factor-alpha (TNF-alpha) and/or interleukin-6 (IL-6) and/or cyclooxygenase-2 (COX-2) and/or interleukin-10 (IL-10).

INVENTOR(S): Dey, Debendranath; Neogi, Partha; Sen, Ananda; Sharma, Somesh D.; Nag, Bishwajit

PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 63 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

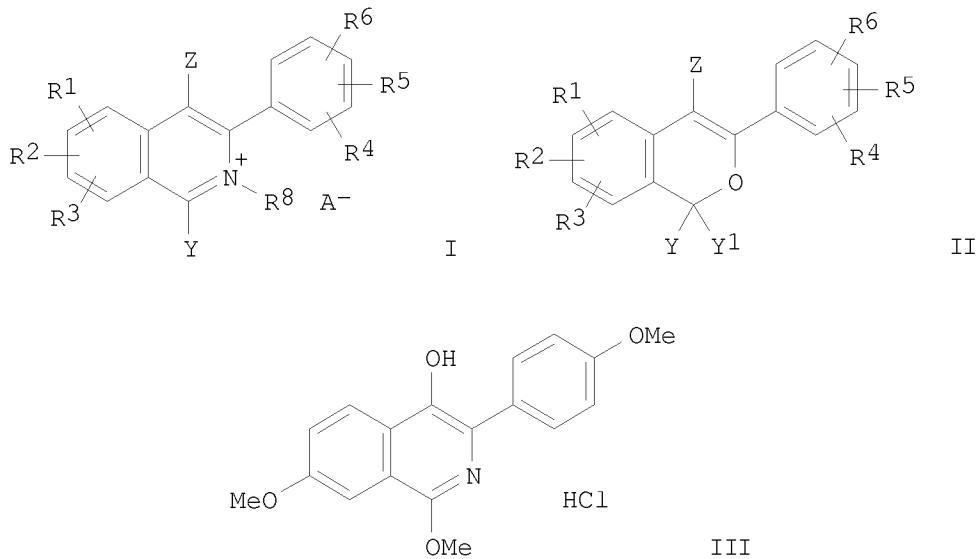
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002030888	A2	20020418	WO 2001-US31731	20011010 <--
WO 2002030888	A3	20020620		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2424292	A1	20020418	CA 2001-2424292	20011010 <--
AU 2002011621	A	20020422	AU 2002-11621	20011010 <--
US 20020077333	A1	20020620	US 2001-973190	20011010 <--
US 6723736	B2	20040420		
EP 1324994	A2	20030709	EP 2001-979686	20011010 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004511465	T	20040415	JP 2002-534276	20011010
PRIORITY APPLN. INFO.:			US 2000-238475P	P 20001010
			WO 2001-US31731	W 20011010

OTHER SOURCE(S): MARPAT 136:309858

GI



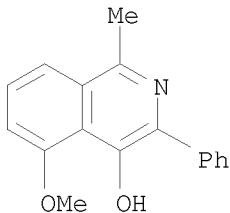
AB Title compds., e.g. [I, II; R1-R6 = H, (substituted) alkyl, alkenyl, aryl, alkylaryl, alkenylaryl, aryl, CO₂R, etc.; R = H, (substituted) alkyl, alkenyl, aryl, Na, K, Ca, Mg, etc.; R8 = H, OH, (substituted) alkyl, alkenyl, aryl, alkylaryl, alkenylaryl, CO₂R, etc.; Y, Y1 = H, (substituted) alkyl, alkenyl, aryl, alkylaryl, alkenylaryl, CO₂R, etc.; Z = OH, (substituted) alkoxy, amino; A- = pharmaceutically acceptable counterion; with provisos], were prepared Thus, a mixture of 2,3-dimethoxybenzylamine, 4-methoxybenzaldehyde, and NaCN was stirred overnight in Me₂CHOH to give 52% isoquinolinone, which was stirred 48 h in aqueous EtOH open to the atmospheric to give 62.8% title compound (III). III at 1-100 μM inhibited LPS-induced IL-6 production in RAW cells by up to 60%.

IT 343779-66-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinolines, isochromanones and isothiochromanones as inhibitors of TNF-α and/or IL-6 and/or COX-2 and/or IL-10)

RN 343779-66-8 HCAPLUS

CN 4-Isoquinolinol, 5-methoxy-1-methyl-3-phenyl- (CA INDEX NAME)

STN



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 11 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:762998 HCAPLUS
DOCUMENT NUMBER: 135:303908
TITLE: 8-(Quinolinylmethyl)xanthine and 8-(isoquinolinylmethyl)xanthine derivatives as PDE 5 inhibitors, useful for treatment of erectile dysfunction
INVENTOR(S): Bhalay, Gurdip; Collingwood, Stephen Paul; Fairhurst, Robin Alec; Gomez, Sylvie Felicite; Naef, Reto; Sandham, David Andrew
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.
SOURCE: PCT Int. Appl., 70 pp.
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077110	A1	20011018	WO 2001-EP3909	20010405 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2403514	A1	20011018	CA 2001-2403514	20010405 <--
AU 2001073921	A	20011023	AU 2001-73921	20010405 <--
EP 1268480	A1	20030102	EP 2001-940294	20010405 <--
EP 1268480	B1	20031105		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001009855	A	20030603	BR 2001-9855	20010405 <--
HU 2003000565	A2	20030728	HU 2003-565	20010405 <--
HU 2003000565	A3	20041028		
JP 2003530398	T	20031014	JP 2001-575583	20010405

STN

JP 3869725	B2	20070117		
AT 253576	T	20031115	AT 2001-940294	20010405
NZ 521361	A	20040528	NZ 2001-521361	20010405
ES 2210169	T3	20040701	ES 2001-940294	20010405
CN 1176922	C	20041124	CN 2001-807489	20010405
AU 2001273921	B2	20050505	AU 2001-273921	20010405
RU 2269529	C2	20060210	RU 2002-129557	20010405
NO 2002004741	A	20021002	NO 2002-4741	20021002 <--
US 20030171384	A1	20030911	US 2002-240481	20021002 <--
ZA 2002007956	A	20030716	ZA 2002-7956	20021003 <--
IN 2002CN01618	A	20050128	IN 2002-CN1618	20021004
MX 2002009903	A	20030327	MX 2002-9903	20021007 <--
US 20040038996	A1	20040226	US 2003-644328	20030820
US 6919337	B2	20050719		
US 20050054660	A1	20050310	US 2004-937639	20040909
US 7019136	B2	20060328		
US 20060173181	A1	20060803	US 2005-274030	20051115
US 20060106214	A1	20060518	US 2006-329889	20060111
US 7361661	B2	20080422		

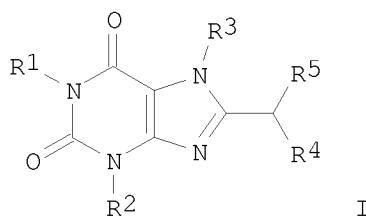
PRIORITY APPLN. INFO.:

GB 2000-8694	A 20000407
WO 2001-EP3909	W 20010405
US 2002-240481	B1 20021002
US 2003-644328	A3 20030820
US 2004-937639	A1 20040909

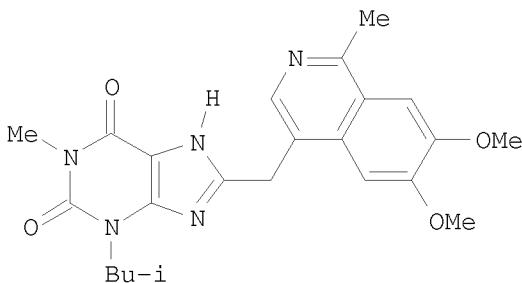
OTHER SOURCE(S) :

MARPAT 135:303908

GI



I



II

AB Compds. of formula I, in free or salt form, are disclosed [where R1 = H or alkyl (un)substituted by OH, alkoxy, or alkylthio; R2 = H, alkyl, hydroxyalkyl, alkylcarbonyloxyalkyl, alkoxyalkyl, alkylthioalkyl, alkenyl, cycloalkylalkyl, heterocyclalkyl, aralkyl [aryl ring optionally fused to

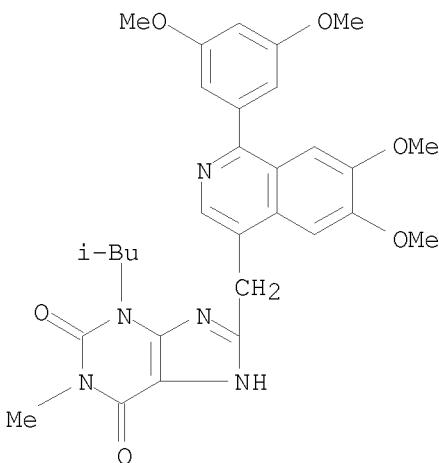
5-membered heterocyclic group or substituted by alkoxy, (di)(alkyl)amino, acylamino, halo, OH, aminosulfonyl, alkylaminosulfonyl, dialkylaminosulfonyl, alkylsulfonylamino or dialkylaminosulfonylamino]; R3 = H or alkyl optionally substituted by OH, alkoxy, or alkylthio; R4 = H or alkyl; R5 = (un)substituted quinolinyl, isoquinolinyl, or oxodihydroisoquinolinyl, optionally fused to 5-membered heterocyclic group [substituents = halo, cyano, OH, alkyl, hydroxylalkyl, alkoxyalkyl, alkylthioalkyl, alkoxy, alkylthio, alkenyl, alkoxy carbonyl, alkynyl, carboxyl, acyl, N(R6)R7, (un)substituted aryl (substituents = halo or alkoxy), or 5- or 6-membered heteroaryl attached through ring C]; R6, R7 = H or alkyl (optionally substituted by OH or alkoxy); or 1 of R6 and R7 = H, the other = acyl; or NR6R7 = 5- or 6-membered heterocyclyl]. I are inhibitors of cGMP phosphodiesterases (PDEs), and in particular are selective inhibitors of PDE5. They exhibit good selectivity for PDE5 over PDE1 and PDE6, indicating a low side-effect profile. I are of particular interest for use in the treatment of sexual dysfunction, especially male erectile dysfunction. Examples include 87 product syntheses and 59 intermediate preps. Ten compds. are particularly preferred, and these are specifically claimed. For instance, cyclocondensation of 5,6-diamino-1-isobutyl-3-methyl-1H-pyrimidine-2,4-dione with (6,7-dimethoxy-1-methylisoquinolin-4-yl)acetic acid (preps. given), using EDC in aqueous MeOH, gave the preferred title compound II. In an in vitro assay

for PDE5 inhibition, I gave IC₅₀ values of 0.0005 μM to 10 μM, e.g., 0.007 μM for II.

IT 366444-39-5P, 8-[6,7-Dimethoxy-1-(3,5-dimethoxyphenyl)isoquinolin-4-ylmethyl]-3-isobutyl-1-methyl-3,7-dihdropurine-2,6-dione
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of quinoline-xanthine and isoquinoline-xanthine derivs. as PDE 5 inhibitors)

RN 366444-39-5 HCPLUS

CN 1H-Purine-2,6-dione, 8-[(1-(3,5-dimethoxyphenyl)-6,7-dimethoxy-4-isoquinolinyl)methyl]-3,9-dihydro-1-methyl-3-(2-methylpropyl)-(CA INDEX NAME)



STN

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 12 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:466987 HCAPLUS

DOCUMENT NUMBER: 135:313435

TITLE: Disease activated drugs: a new concept for the treatment of asthma

AUTHOR(S): Charpiot, B.; Bitsch, F.; Buchheit, K.-H.; Channez, P.; Mazzoni, L.; Mueller, T.; Vachier, I.; Naef, R.

CORPORATE SOURCE: Research, Novartis Pharma AG, Basel, CH-4002, Switz.

SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(7), 1793-1805

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:313435

AB Disease activated drugs (DAD) are pro-drugs of one active principle or combinations of two drugs, which have a proven efficacy for the treatment of the target disease. In opposition to pro-drugs, DAD are activated in inflamed but not normal tissues. Due to the disease specific activation, the amount of locally released drug(s) should be related directly to the severity of the inflammation. To test this concept in asthma a PDE4 inhibitor, an isoquinoline derivative, was chemical derivatized into pro-drugs

or

combined with corticosteroids. These new compds. were more readily cleaved into active PDE4 inhibitor, in bronchoalveolar lavage fluid (BALF) from Brown-Norway rats with lung inflammation than in BALF from rats without airway inflammation. The DAD concept (local selective release and improved therapeutic window) was validated in vivo using the inhibition of methacholine induced bronchoconstriction in guinea pigs with or without ozone induced lung inflammation. An example of DAD hydrolysis (isoquinoline-dexamethasone) was also examined in BALF from asthmatics and healthy volunteers. PDE4 inhibitors derivatized or combined with steroids were synthesized as DAD models and their cleavage into active PDE4 inhibitors under inflammatory conditions were examined in vitro. The DAD concept was also validated in animals, local release and improved therapeutic window were observed

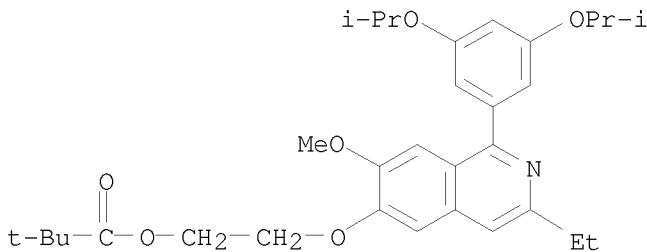
IT 368445-15-2P

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); USES (Uses); PROC (Process); USES (Uses)

(preparation of disease activated drugs that inhibit phosphodiesterase type 4 as a new concept for the treatment of asthma)

RN 368445-15-2 HCAPLUS

CN Propanoic acid, 2,2-dimethyl-, 2-[1-[3,5-bis(1-methylethoxy)phenyl]-3-ethyl-7-methoxy-6-isoquinolinyl]oxy]ethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
 (6 CITINGS)
 REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 13 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2001:136925 HCAPLUS
 DOCUMENT NUMBER: 134:188213
 TITLE: Treatment of obstructive airways diseases with compositions comprising propylsulfonylethylaminoethyl benzothiazolone and PDE4 inhibitors
 INVENTOR(S): Ince, Francis; Dixon, John; Holt, Philip
 PATENT ASSIGNEE(S): AstraZeneca UK Limited, UK
 SOURCE: PCT Int. Appl., 14 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001011933	A2	20010222	WO 2000-GB3114	20000814 <--
WO 2001011933	A3	20010614		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000064602	A	20010313	AU 2000-64602	20000814 <--
PRIORITY APPLN. INFO.:			SE 1999-2937	A 19990818
			WO 2000-GB3114	W 20000814

AB The present invention provides a pharmaceutical composition, pharmaceutical product or kit comprising a first active ingredient (A) being 4-hydroxy-7-[2-[2-[3-[2-phenylethoxy]propylsulfonyl]ethylamino]ethyl]-1,3-benzothiazol-2(3H)-one (I) or a pharmaceutically acceptable salt thereof, and a second active ingredient (B) being a PDE4 inhibitor, for use in the treatment of obstructive airways diseases. Antiinflammatory efficacy of a combination of 10 mg/kg oral ariflo and 0.3 g/kg aerosol I was shown in rats.

IT 125175-65-7
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological

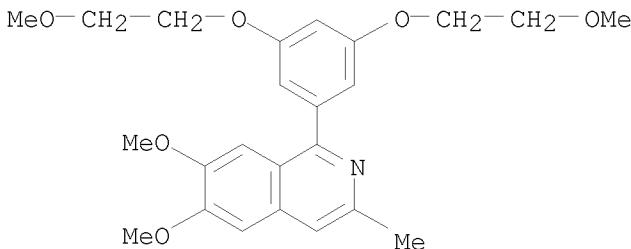
STN

study, unclassified); THU (Therapeutic use); BIOL (Biological study);
USES (Uses)

(treatment of obstructive airways diseases with compns. comprising
propylsulfonylethylaminoethyl benzothiazolone and PDE4 inhibitors)

RN 125175-65-7 HCPLUS

CN Isoquinoline, 1-[3,5-bis(2-methoxyethoxy)phenyl]-6,7-dimethoxy-3-methyl-
(CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 14 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:712977 HCPLUS

DOCUMENT NUMBER: 133:281699

TITLE: Preparation of isoquinoline derivatives as
phosphodiesterase V inhibitors

INVENTOR(S): Ukita, Shinzo; Yamada, Koichiro; Ohmori, Kenji;
Yoshikawa, Kohei

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 49 pp.

CODEN: JKXXAF

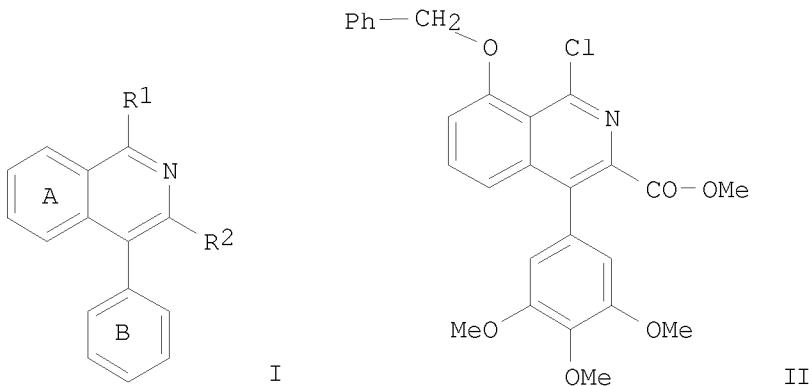
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

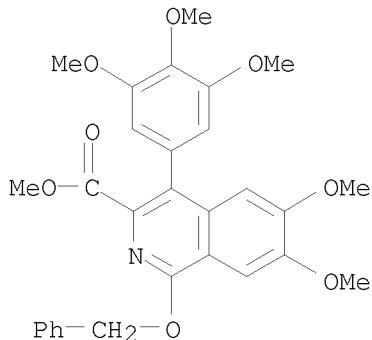
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000281654	A	20001010	JP 1999-83022	19990326 <--
PRIORITY APPLN. INFO.:			JP 1999-83022	19990326
OTHER SOURCE(S):	MARPAT	133:281699		
GI				



AB The title compds. I [ring A = benzene ring with substituents; ring B = (un)substituted benzene ring; R1 = (un)substituted alkoxy, halo, etc.; R2 = CO₂R₃, etc.; R₃ = H, etc.], useful as phosphodiesterase V inhibitors (no data) for the treatment of circulatory system diseases (no data), are prepared. For example, the title compound II was prepared
IT 299167-15-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinoline derivs. as phosphodiesterase V inhibitors)
RN 299167-15-0 HCPLUS
CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-(phenylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)

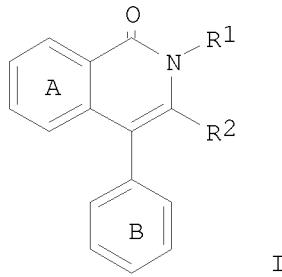


L14 ANSWER 15 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2000:151451 HCPLUS
 DOCUMENT NUMBER: 132:207769
 TITLE: Preparation of isoquinolinones as effective component in medicine
 INVENTOR(S): Ukita, Shinzo; Ohmori, Kanji; Ikeo, Tomihiro
 PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 148 pp.
 CODEN: JKXXAF

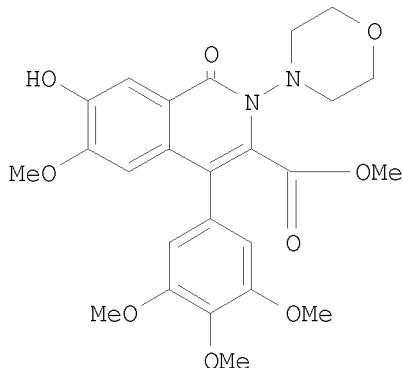
STN

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000072675	A	20000307	JP 1998-240446	19980826 <--
PRIORITY APPLN. INFO.:			JP 1998-240446	19980826
OTHER SOURCE(S):	MARPAT	132:207769		
GI				



I



II

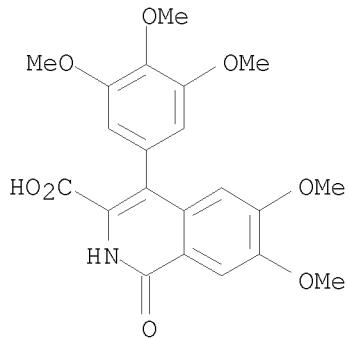
AB Title compds. [I; ring A and ring B equivalent or different, substituted or unsubstituted benzene ring; R1 = H, N(CH₃)₂, 4-H₂NC₆H₄, 4-CH₃OCOC₆H₄, alkyl, cycloalkyl, aryl, complex cyclic; R2 = COOH, COOCH₃, COOCH₂CH₃, COOCH₂C₆H₅, COO(CH₂)₃CH₃] and pharmaceutical acceptable salts are prepared and tested as PDEV inhibitors. The title compound II was prepared

IT 212489-07-1P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinolinones as effective component in medicine)

RN 212489-07-1 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)

STN



L14 ANSWER 16 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:137239 HCPLUS

DOCUMENT NUMBER: 132:194292

TITLE: Preparation of medicine composition containing pyridylamines

INVENTOR(S): Ukita, Tatsuzo; Sugawara, Masakatsu; Ikezawa, Ichiro; Yoshikawa, Hideo; Naito, Kazuaki

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 41 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000063275	A	20000229	JP 1999-164565	19990611 <--
PRIORITY APPLN. INFO.:			JP 1998-164045	A 19980612
OTHER SOURCE(S):	MARPAT	132:194292		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

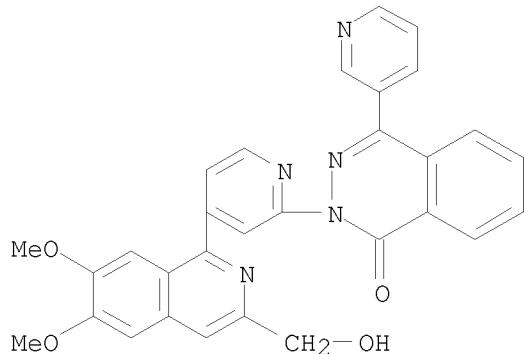
AB Title compds. [I; Q = N containing substituted benzoheterocyclic ring; Q1 = N containing substituted benzoheterocyclic ring], stereoisomers, pharmaceutical acceptable salts are prepared as active components in antiasthmatics. The title compound II was prepared

IT 209261-39-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridylamines as antiasthmatics)

RN 209261-39-2 HCPLUS

CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-isoquinolinyl]-2-pyridinyl]-4-(3-pyridinyl)-, hydrochloride (1:1) (CA INDEX NAME)

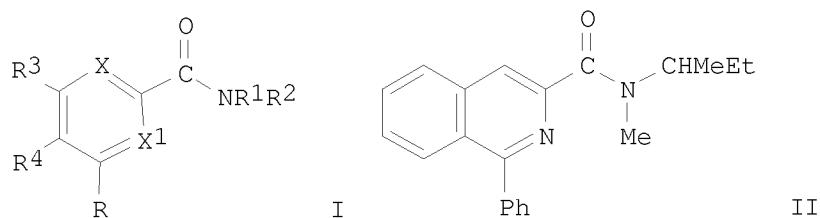


● HCl

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L14 ANSWER 17 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:732901 HCAPLUS
DOCUMENT NUMBER: 131:310567
TITLE: Arene- and heteroarenenecarboxamides as benzodiazepine receptors
INVENTOR(S): Dubroeucq, Marie-Christine; Renault, Christian; Le Fur, Gerard
PATENT ASSIGNEE(S): Pharmuka Laboratoires, Fr.
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4499094	A	19850212	US 1983-482082	19830405 <--
FR 2525595	A1	19831028	FR 1982-7217	19820427 <--
FR 2525595	B1	19850322		
PRIORITY APPLN. INFO.:			FR 1982-7217	A 19820427
GI				



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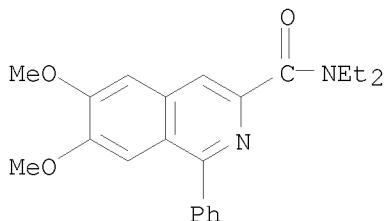
AB Carboxamides I [X, X1 = N, CH; R = Ph, substituted Ph, pyridyl, thienyl; R1, R2 = aliphatic, aromatic; NR1R2 = heterocyclic; R3R4 = (un)substituted CH:CHCH:CH, SCH:CH, CH:CHS] were prepared. Thus 2.4 g II was obtained by amidating 2.96 g of acid with 1.34 g MeNHCHMeEt. II had an affinity for benzodiazepine receptors of 2 nM. The compds. are useful as medicaments for the various applications of benzodiazepines.

IT 89242-44-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and affinity for benzodiazepine receptor)

RN 89242-44-4 HCPLUS

CN 3-Isoquinolinecarboxamide, N,N-diethyl-6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 18 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:244638 HCPLUS

DOCUMENT NUMBER: 130:311813

TITLE: Preparation of piperazinylisoquinolines and analogs as serotonin antagonists

INVENTOR(S): Ueno, Kohshi; Sasaki, Atsushi; Kawano, Koki; Okabe, Tadashi; Kitazawa, Noritaka; Takahashi, Keiko; Yamamoto, Noboru; Suzuki, Yuichi; Matsunaga, Manabu; Kubota, Atsuhiko

PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan

SOURCE: PCT Int. Appl., 740 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9918077	A1	19990415	WO 1998-JP4465	19981002 <--
W: US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2000053647	A	20000222	JP 1998-281752	19981002 <--
JP 3989102	B2	20071010		

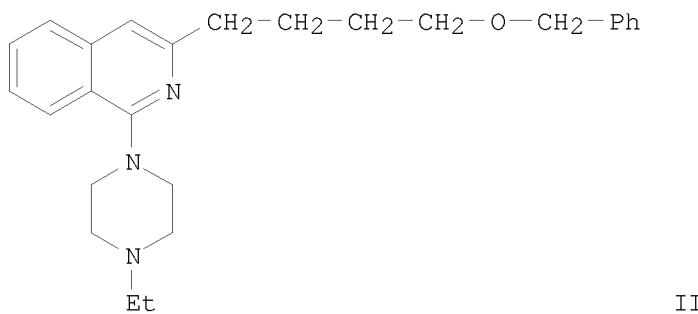
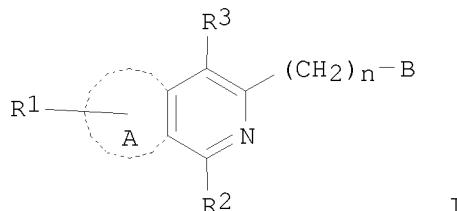
STN

EP 1020445	A1	20000719	EP 1998-945593	19981002 <--
EP 1020445	B1	20080813		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				

AT 404539	T	20080815	AT 1998-945593	19981002
US 6340759	B1	20020122	US 2000-509778	20000331 <--
US 20020013460	A1	20020131	US 2001-852850	20010511 <--
US 6790844	B2	20040914		
US 20040204421	A1	20041014	US 2004-796673	20040310
US 6875761	B2	20050405		

PRIORITY APPLN. INFO.:				
		JP 1997-284290	A 19971002	
		JP 1998-153416	T0 19980602	
		WO 1998-JP4465	W 19981002	
		US 2000-509778	A3 20000331	
		US 2001-852850	A3 20010511	

OTHER SOURCE(S): MARPAT 130:311813
GI

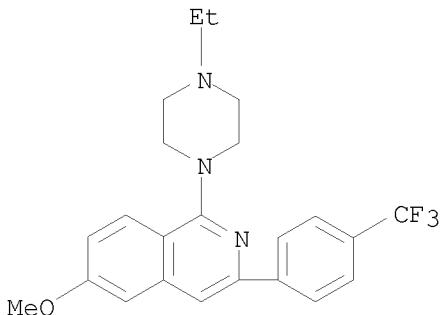


AB The title compds. I [ring A = benzene, pyridine, thiophene or furan ring; B = (un)substituted aryl, etc.; R1 = H, halo, etc.; R2 = 4-morpholinyl, etc.; R3 = H, halo, etc.; n = 0, or 1 - 6] are prepared I are central muscle relaxing drugs for treating, ameliorating or preventing spastic paralysis or ameliorating myotonia. In an in vitro test for 5HT1 receptor antagonism, the title compound II showed the Ki value of 21.2 nM.

IT 223544-97-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperazinylisoquinolines and analogs as serotonin

STN

antagonists)
RN 223544-97-6 HCPLUS
CN Isoquinoline, 1-(4-ethyl-1-piperazinyl)-6-methoxy-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

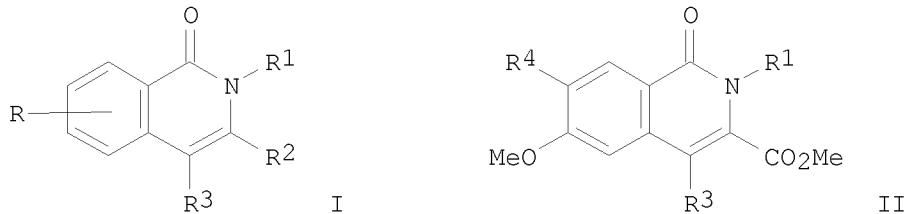
L14 ANSWER 19 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:608601 HCPLUS
DOCUMENT NUMBER: 129:216521
ORIGINAL REFERENCE NO.: 129:44019a, 44022a
TITLE: Preparation of 1-isoquinolinone-3-carboxylates as PDE V inhibitors
INVENTOR(S): Ukita, Tatsuzo; Omori, Kenji; Ikeo, Tomihiro
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 299 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9838168	A1	19980903	WO 1998-JP715	19980223 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 1998MA00345	A	20050304	IN 1998-MA345	19980220
AU 9862300	A	19980918	AU 1998-62300	19980223 <--
JP 10298164	A	19981110	JP 1998-44139	19980226 <--
PRIORITY APPLN. INFO.:			JP 1997-44408	A 19970227
			WO 1998-JP715	W 19980223

OTHER SOURCE(S): MARPAT 129:216521

STN

GI



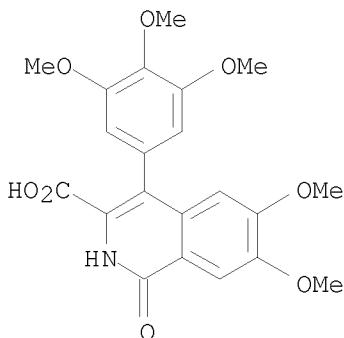
AB Title compds. [I; R = H or substituent(s); R¹ = H, NH₂, (cyclo)alkyl, heterocyclyl, aryl, etc.; R² = (esterified) CO₂H, CONH₂, N-attached heterocyclylcarbonyl, etc.; R³ = (un)substituted Ph] were prepared as PDE V inhibitors (no data). Thus, 5-benzylbenzoic acid was cyclocondensed with CH₂(CO₂CMe₃)₂ and the hydrated product cyclocondensed with 4-(H₂N)C₆H₄NHCO₂CMe₃ to give, in 4 addnl. steps, title compound II [R¹ = C₆H₄(NH₂)-4, R³ = C₆H₂(OMe)₃-3,4,5, R⁴ = 2-pyridylmethoxy].

IT 212489-07-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 1-isooquinolinone-3-carboxylates as PDE V inhibitors)

RN 212489-07-1 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 20 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:398243 HCPLUS
DOCUMENT NUMBER: 129:81741

STN

ORIGINAL REFERENCE NO.: 129:16880h,16881a
TITLE: Preparation of pyridines as antiasthmatics
INVENTOR(S): Ukita, Tatsuzo; Sugahara, Masakatsu; Ikezawa, Katsuo;
Kikkawa, Hideo; Naito, Kazuaki
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 59 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 848000	A1	19980617	EP 1997-309947	19971210 <--
EP 848000	B1	20020612		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 5965730	A	19991012	US 1997-985042	19971204 <--
TW 429257	B	20010411	TW 1997-86118300	19971205 <--
AT 219075	T	20020615	AT 1997-309947	19971210 <--
ES 2178741	T3	20030101	ES 1997-309947	19971210 <--
CA 2224635	A1	19980613	CA 1997-2224635	19971211 <--
CA 2224635	C	20060131		
CN 1184813	A	19980617	CN 1997-125491	19971212 <--
CN 1127498	C	20031112		
JP 10226685	A	19980825	JP 1997-342352	19971212 <--
JP 3951395	B2	20070801		
HK 1012505	A1	20021025	HK 1998-113891	19981217 <--
PRIORITY APPLN. INFO.:			JP 1996-333357	A 19961213
OTHER SOURCE(S):	MARPAT	129:81741		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

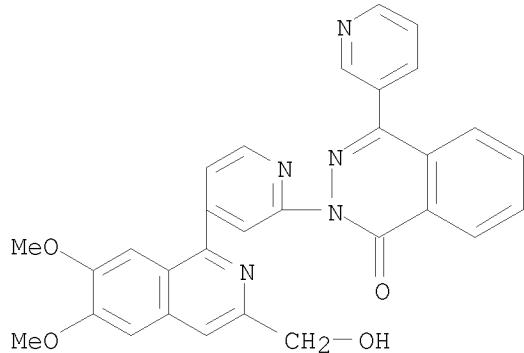
AB The title compds. [I; A = II-VI (wherein R₁, R₂ = H, (un)protected OH; R₃₁, R₄₁, R₄₂ = (un)protected CH₂OH; R₃₂ = H, lower alkyl, (un)protected CH₂OH; R₃₃ = (un)substituted lower alkyl; the dotted line means the presence or absence of a double bond); R₅, R₆ = H, (un)protected NH₂, or NR₅R₆ = (un)substituted heterocycle], which show excellent bronchoconstriction inhibitory activity and/or anti-inflammatory activity of airways, and therefore are useful in the prophylaxis or treatment of asthma, were prepared. Thus, reaction of 4-(3-pyridyl)phthalazin-1(2H)-one with 2-bromo-4-[6,7-dimethoxy-2-(4-pyridyl)methyl]phthalazin-1(2H)-one-4-yl]pyridine in the presence of K₂CO₃ and CuI in DMF afforded the title compound VII. Compds. I are effective at 0.003-3 mg/kg/day.

IT 209261-38-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridines as antiasthmatics)

RN 209261-38-1 HCPLUS
CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-

STN

isoquinolinyl]-2-pyridinyl]-4-(3-pyridinyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(16 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

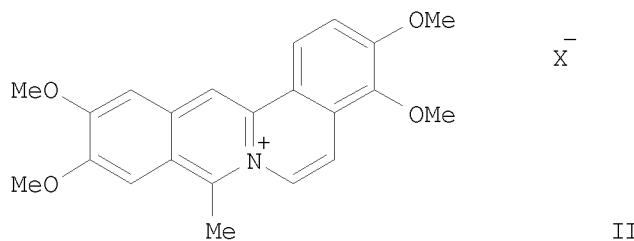
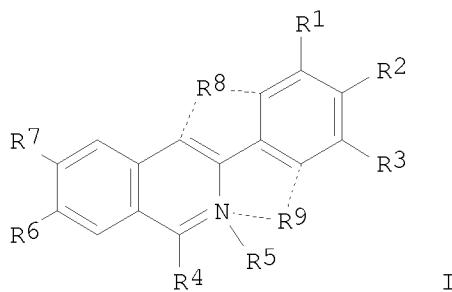
L14 ANSWER 21 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:542447 HCAPLUS
DOCUMENT NUMBER: 127:220851
ORIGINAL REFERENCE NO.: 127:43049a,43052a
TITLE: Coralynne analogs as topoisomerase inhibitors
INVENTOR(S): Lavoie, Edmond J.
PATENT ASSIGNEE(S): Rutgers, State University of New Jersey, USA; Lavoie,
Edmond J.
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9729106	A1	19970814	WO 1997-US1676	19970211 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2241551	A1	19970814	CA 1997-2241551	19970211 <--
AU 9721155	A	19970828	AU 1997-21155	19970211 <--
AU 710070	B2	19990916		
EP 888346	A1	19990107	EP 1997-906466	19970211 <--
EP 888346	B1	20010606		
R: BE, DE, ES, FR, GB, IT, NL, SE, PT				
CN 1211252	A	19990317	CN 1997-192211	19970211 <--
CN 1067070	C	20010613		

STN

HU 9900413	A2	19990528	HU 1999-413	19970211 <--
HU 9900413	A3	20020228		
BR 9707425	A	19990720	BR 1997-7425	19970211 <--
NZ 330705	A	20000327	NZ 1997-330705	19970211 <--
JP 2000504687	T	20000418	JP 1997-528606	19970211 <--
ES 2161442	T3	20011201	ES 1997-906466	19970211 <--
US 6121275	A	20000919	US 1998-117558	19980731 <--
NO 9803669	A	19980923	NO 1998-3669	19980811 <--
PRIORITY APPLN. INFO.:			US 1996-11452P	P 19960212
			US 1996-32161P	P 19961001
			WO 1997-US1676	W 19970211

OTHER SOURCE(S): MARPAT 127:220851
GI

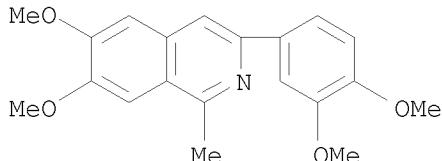


AB The coralyne derivs. I (R1, R2, R3, R6, R7 = H, OH, alkoxy, R2R3 and R6R7 may form OCH₂O; R4, R5 = H, alkyl; R8, R9 = CH:CH, CH₂CH₂, or ar absent) were prepared as anticancer agents and topoisomerase inhibitors. Thus, the dibenzoquinolizinium derivative II (X = acetosulfate) was pred. in 4 steps. starting from 2,3-dimethoxyphenethylamine and 3,4-dimethoxyacetyl chloride. via cyclization of N-(2,3-dimethoxyphenethyl)-2-(3,4-dimethoxyphenyl)acetamide and 5,6-dimethoxy-1-(3,4-dimethoxybenzyl)isoquinoline hydrochloride. The cytotoxicity IC₅₀ of II (X = acetosulfate) against RPMI cell lines was .4 μM.

IT 35989-93-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); USES (Uses); RACT

STN

(Reactant or reagent); USES (Uses)
(preparation of Coralyne analogs as topoisomerase inhibitors)
RN 35989-93-6 HCAPLUS
CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 22 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:432292 HCAPLUS
DOCUMENT NUMBER: 125:131653
ORIGINAL REFERENCE NO.: 125:24329a,24332a
TITLE: Coralyne and related compounds as mammalian topoisomerase I and topoisomerase II poisons
AUTHOR(S): Makhey, Darshan; Gatto, Barbara; Yu, Chiang; Liu, Angela; Liu, Leroy F.; LaVoie, Edmond J.
CORPORATE SOURCE: Dep. Pharmaceutiactl Chem., Rutgers, State Univ. New Jersey, Piscataway, NJ, 08855, USA
SOURCE: Bioorganic & Medicinal Chemistry (1996), 4(6), 781-791
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB DNA topoisomerases are nuclear enzymes responsible for modifying the topol. state of DNA. The development of agents capable of poisoning topoisomerases has proved to be an attractive approach in the search for novel cancer chemotherapeutics. Coralyne, an antileukemic alkaloid, has appreciable structural similarity to the potent topoisomerase I and II position, nitidine. Analogs of coralyne were synthesized and evaluated for their activity as topoisomerase I and topoisomerase II poisons. These analogs were also evaluated for cytotoxicity in the human lymphoblast cell line, RPMI 8402, and its camptothecin-resistant variant, CPT-K5. The pharmacol. activity of these analogs exhibited a strong dependence on the substitution pattern and the nature of substituents. Several 1-benzylisoquinolines and 3-phenylisoquinolines were also synthesized. These compds., which incorporate only a portion of the ring structure of coralyne, were evaluated as topoisomerase poisons and for cytotoxicity. These structure-activity studies indicate that the structural rigidity associated with the coralyne ring system may be critical for pharmacol. activity. The presence of a 3,4-methylenedioxy substituent on these coralyne analogs was generally associated with enhanced activity as a topoisomerase poison. 5,6-Dihydro-3,4-methylenedioxy-10,11-dimethoxydibenzo[a,g]quinolizinium chloride was the most potent

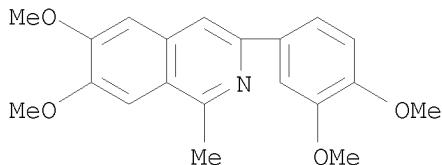
topoisomerase I poison among the coralyne analogs evaluated, having similar activity to camptothecin. This analog also possessed exceptional potency as a topoisomerase II poison. Despite the pronounced activity of several of these coralyne derivs. as topoisomerase I poisons, none of these compds. had cytotoxic activity similar to camptothecin. Possible differences in cellular absorption between these coralyne analogs, which possess a quaternary ammonium group, and camptothecin may be responsible for the differences observed in their relative cytotoxicity.

IT 35989-93-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-activity relations of coralyne analogs as topoisomerase I and II poison and cytotoxic agents)

RN 35989-93-6 HCAPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 48 THERE ARE 48 CAPLUS RECORDS THAT CITE THIS RECORD (48 CITINGS)

L14 ANSWER 23 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:206265 HCAPLUS

DOCUMENT NUMBER: 124:307215

ORIGINAL REFERENCE NO.: 124:56647a, 56650a

TITLE: Cyclic AMP promotes the survival of dopaminergic neurons in vitro and protects them from the toxic effects of MPP⁺

AUTHOR(S): Hulley, P.; Hartikka, J.; Lubbert, H.

CORPORATE SOURCE: Preclinical Research, Sandoz Pharma Ltd, Basel, Switz.

SOURCE: Journal of Neural Transmission, Supplement (

1995), 46(Parkinsons Disease: Experimental

Models and Therapy), 217-28

CODEN: JNTSD4; ISSN: 0303-6995

PUBLISHER: Springer

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors have studied how stimulation of protein kinase C and cAMP-dependent protein kinases affect the development of mesencephalic dopaminergic neurons in vitro. Insulin-like growth factor-I (IGF-I) and basic fibroblast growth factor (bFGF) did not activate either second messenger system nor affect the survival of dopaminergic neurons but stimulated average dopamine uptake per neuron. Phorbol esters, which stimulate protein kinase C, had no effect on dopamine uptake. Dibutyryl-cAMP caused an increase in dopamine uptake, which was blocked with (Rp)-cAMPS, a specific inhibitor of cAMP-dependent protein kinases. Treating cells with specific phosphodiesterase type IV inhibitors elevated

the forskolin-induced increase in dopamine uptake. Furthermore, cAMP, but neither bFGF nor activation dependent astrocyte factor (ADAF), was able to prevent the degeneration of dopaminergic neurons induced by MPP+. These results suggest that increased intracellular cAMP protects dopaminergic neurons in situations of stress and therefore reveal novel possibilities for the treatment of Parkinson's disease.

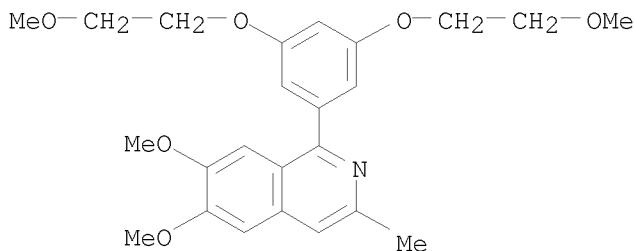
IT 125175-65-7, SDZ-MNS 949

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(increasing cAMP and neurotrophic factors promote survival of mesencephalic dopaminergic neuron cultures in vitro and protects them from toxic effects of MPP+ in relation to protein kinases and Parkinson's disease treatment)

RN 125175-65-7 HCAPLUS

CN Isoquinoline, 1-[3,5-bis(2-methoxyethoxy)phenyl]-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L14 ANSWER 24 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:720049 HCAPLUS

DOCUMENT NUMBER: 123:188478

ORIGINAL REFERENCE NO.: 123:33241a,33244a

TITLE: Mechanism of antioxidant action of screened phenols in biological membranes. Antioxidant action of ionols "in vivo". The protective effects of lipo- and water-soluble ionol antioxidants on the cytochrome P-450 system of liver microsome membranes during lipid peroxidation

AUTHOR(S): Savov V.; Harfouf, Mahammed

CORPORATE SOURCE: Lab. Biofiz. Biomembr., Fak. Fiz., Sofia, Bulg.

SOURCE: Godishnik na Sofiiskiya Universitet "Sv. Kliment Okhridski", Fizicheski Fakultet (1995),

Volume Date 1994, 86, 145-53

CODEN: GSUFA3; ISSN: 0584-0279

PUBLISHER: Universitetsko Izdatelstvo Sv. Kliment Okhridski

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The effect of ionols on the lipid peroxidn. "in vivo", induced by nonenzymic system Fe²⁺-ascorbic acid in the homogenates of rat liver and brain is studied. Relative differences in the activities of ionols are discussed. The protective effects of ionols on monooxygenase system

STN

during lipid peroxidn. in liver microsome membranes were studied. It was shown that some of these liposol. antioxidants have optimal protection effect on cytochrome P 450.

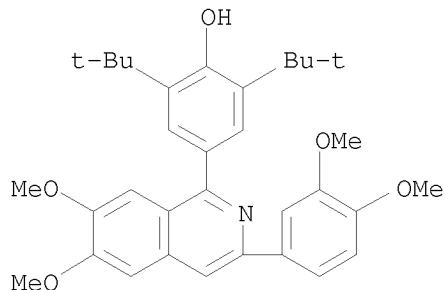
IT 132054-21-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(protective effects of lipo- and water-soluble ionol antioxidants on liver cytochrome P 450 system during lipid peroxidn.)

RN 132054-21-8 HCAPLUS

CN Phenol, 4-[3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-isoquinolinyl]-2,6-bis(1,1-dimethylethyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L14 ANSWER 25 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:621790 HCAPLUS

DOCUMENT NUMBER: 123:32971

ORIGINAL REFERENCE NO.: 123:6095a

TITLE: Isoquinolines for asthma therapy

INVENTOR(S): Naef, Reto

PATENT ASSIGNEE(S): Sandoz-Patent-GmbH, Germany

SOURCE: Ger. Offen., 14 pp.

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4438737	A1	19950511	DE 1994-4438737	19941029 <--
FR 2711989	A1	19950512	FR 1994-13108	19941028 <--
FR 2711989	B1	19960614		
CH 688478	A5	19971015	CH 1994-3226	19941028 <--
GB 2283488	A	19950510	GB 1994-21985	19941101 <--
GB 2283488	B	19971203		
EP 664289	A2	19950726	EP 1994-810628	19941101 <--
EP 664289	A3	19950913		

R: BE, DK, ES, GR, IE, LU, NL, PT, SE

STN

CA 2135000	A1	19950506	CA 1994-2135000	19941103 <--
FI 9405191	A	19950506	FI 1994-5191	19941103 <--
NO 9404187	A	19950508	NO 1994-4187	19941103 <--
AU 9477610	A	19950518	AU 1994-77610	19941103 <--
AU 685852	B2	19980129		
CZ 282329	B6	19970611	CZ 1994-2698	19941103 <--
IL 111518	A	19990620	IL 1994-111518	19941103 <--
SK 280298	B6	19991108	SK 1994-1319	19941103 <--
JP 07188176	A	19950725	JP 1994-271172	19941104 <--
CN 1106801	A	19950816	CN 1994-118199	19941104 <--
CN 1051998	C	20000503		
HU 71350	A2	19951128	HU 1994-3184	19941104 <--
HU 217120	B	19991129		
ZA 9408738	A	19960506	ZA 1994-8738	19941104 <--
AT 9402048	A	19980815	AT 1994-2048	19941104 <--
AT 404940	B	19990325		
RU 2144027	C1	20000110	RU 1994-40170	19941104 <--
PL 178210	B1	20000331	PL 1994-305705	19941104 <--
US 5747506	A	19980505	US 1996-771556	19961220 <--
PRIORITY APPLN. INFO.:			GB 1993-22828	A 19931105
			US 1994-333699	B1 19941103
			US 1995-472042	B1 19950606

OTHER SOURCE(S): CASREACT 123:32971; MARPAT 123:32971
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

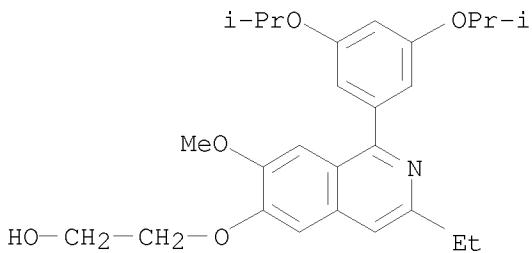
AB Title compds. I [R = Et, Pr] and their physiol. acceptable/hydrolyzable esters and/or acid addition salts are claimed. The compds. are useful for treatment of obstructive or inflammatory airway diseases, especially asthma. For example, isovanillin underwent etherification with PhCH₂OCH₂CH₂I, followed by Darzens-type condensation with EtCHBrCO₂Et and hydrolysis/decarboxylation/rearrangement of the product, to give 3-(2-benzyloxyethoxy)-4-methoxybenzyl Et ketone (II). This underwent reductive amination with NH₄OAc and NaBH₃CN, amidation of the formed amine with 3,5-diisopropoxybenzoyl chloride, and cyclization of the amide with POCl₃ in refluxing MeCN, to give dihydroquinoline derivative III. This was simultaneously dehydrogenated and hydrogenolytically deprotected by heating with 10% Pd/C in decalin at 200°, giving I (R = Et). I showed selectivity for inhibition of type IV PDE isoenzyme, and showed activity in a variety of tests, including inhibition of TNF- α secretion, inhibition of SRS-A formation, relaxation of isolated human bronchus, inhibition of chemical and biol. induced bronchoconstriction, and addnl. tests for immunosuppression.

IT 163923-99-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinolines for asthma therapy)

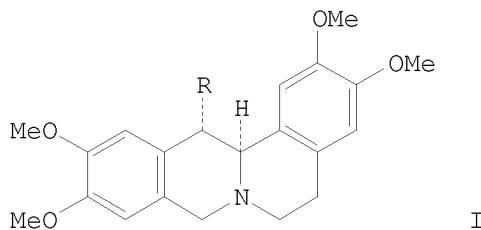
RN 163923-99-7 HCPLUS

CN Ethanol, 2-[(1-[3,5-bis(1-methylethoxy)phenyl]-3-ethyl-7-methoxy-6-isoquinolinyl]oxy]- (CA INDEX NAME)

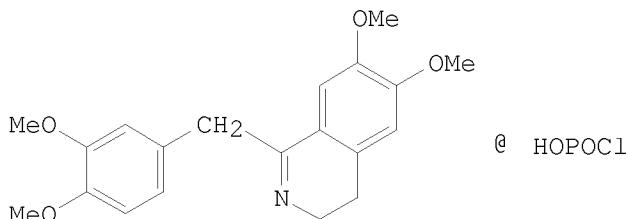


OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

L14 ANSWER 26 OF 29 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:165652 HCAPLUS
DOCUMENT NUMBER: 110:165652
ORIGINAL REFERENCE NO.: 110:27249a, 27252a
TITLE: 2,3,10,11-Tetramethoxy-5,6,7,8,13,13a -
hexahydroprotoberberines and their B-seco analogs:
synthesis and antineoplastic activity
AUTHOR(S): Sladkov, V. I.; Sazonova, N. M.; Grekova, G. S.;
Kalistratov, S. G.; Sokolova, A. S.; Chernov, V. A.;
Suvorov, N. N.
CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst. im. Mendeleeva, Moscow,
USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1989),
23(1), 50-3
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 110:165652
GI



I



II

STN

AB (\pm)-Xylopinine (I, R = H) and (\pm)-13 α -hydroxyxylopinine (I, R = OH) were prepared by the oxidation of II with O in alkaline medium followed by

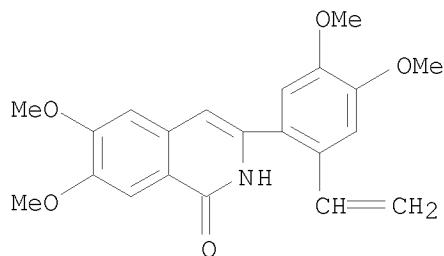
NaBH4 reduction and Pictet-Spengler cyclization of the resulting erythro-(\pm)- α -hydroxynorlaudanosine [for I (R = OH)] or by the NaBH4 reduction of II to (\pm)-norlaudanosine followed by Pictet-Spengler cyclization [for (\pm)-xylopinine]. Other derivs. of I were also synthesized. (\pm)-Xylopinine and its quaternary ammonium seco analog were toxic at ≥ 200 mg/kg in rats. All the compds. showed antitumor activity, with the most active being (\pm)-xylopinine. Seco analogs were less active.

IT 60315-12-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antitumor activity of)

RN 60315-12-0 HCPLUS

CN 1(2H)-Isoquinolinone, 3-(2-ethenyl-4,5-dimethoxyphenyl)-6,7-dimethoxy-
(CA INDEX NAME)



L14 ANSWER 27 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1988:422849 HCPLUS

DOCUMENT NUMBER: 109:22849

ORIGINAL REFERENCE NO.: 109:3904h,3905a

TITLE: Preparation of 3-(hydroxymethyl)isoquinolines as cardiotonics

INVENTOR(S): Rabloczky, Gyorgy; Korosi, Jeno; Lang, Tibor; Ling, Istvan; Hamori, Tamas; Kuhar, Maria; Elekes, Istvan; Botka, Peter; Varro, Andras; et al.

PATENT ASSIGNEE(S): EGIS Gyogyszergyar, Hung.

SOURCE: Brit. UK Pat. Appl., 17 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

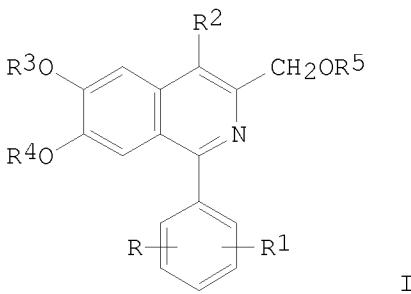
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2190678	A	19871125	GB 1987-12047	19870521 <--
GB 2190678	B	19900620		
HU 44017	A2	19880128	HU 1986-2141	19860521 <--
HU 196758	B	19890130		

CH 673280	A5	19900228	CH 1987-1917	19870519 <--
US 4785104	A	19881115	US 1987-51767	19870520 <--
DK 8702582	A	19871122	DK 1987-2582	19870521 <--
FI 8702256	A	19871122	FI 1987-2256	19870521 <--
SE 8702119	A	19871122	SE 1987-2119	19870521 <--
FR 2599033	A1	19871127	FR 1987-7119	19870521 <--
NL 8701214	A	19871216	NL 1987-1214	19870521 <--
DE 3717079	A1	19880107	DE 1987-3717079	19870521 <--
JP 63039863	A	19880220	JP 1987-124993	19870521 <--
ES 2005583	A6	19890316	ES 1987-1497	19870521 <--
BE 1000719	A4	19890321	BE 1987-572	19870521 <--
CS 264293	B2	19890613	CS 1987-3691	19870521 <--
DD 268940	A5	19890614	DD 1987-303003	19870521 <--
SU 1551245	A3	19900315	SU 1987-4202630	19870521 <--
PRIORITY APPLN. INFO.:			HU 1986-2141	A 19860521

OTHER SOURCE(S):

MARPAT 109:22849

GI



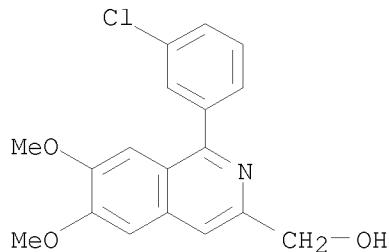
AB The title compds. I (R, R1 = H, halo, NO₂, C1-4 alkoxy; R2, R3, R4 = C1-4 alkyl; R₃R₄ = CH₂; R₅ = H) were prepared by hydrolysis of I (R₅ = acyl). 1-(3,4-Dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisoquinoline N-oxide was refluxed with Ac₂O 2.5 h to give 84.1% I (R = 3-MeO, R₁ = 4-MeO, R₂ = Et, R₃ = R₄ = Me, R₅ = Ac). Similarly prepared I (R = 3-Cl, R₁ = R₂ = H, R₃ = R₄ = Me, R₅ = Ac) was refluxed in 5% aqueous HCl to give 82.4% I.HCl (R = 3-Cl, R₁ = R₂ = R₅ = H, R₃ = R₄ = Me) (II) which, at 5 mg/kg i.v., gave a 50% increase in myocardial contractile force in anesthetized open-chest cats. Tablets were prepared containing II 10, lactose 185, cellulose 25, talc 5, starch 73, and Mg stearate 2 g per 103.

IT 114919-85-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as cardiotonic)

RN 114919-85-6 HCPLUS

CN 3-Isoquinolinemethanol, 1-(3-chlorophenyl)-6,7-dimethoxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L14 ANSWER 28 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1988:186593 HCPLUS

DOCUMENT NUMBER: 108:186593

ORIGINAL REFERENCE NO.: 108:30654h, 30655a

TITLE: Preparation and formulation of 4-N-substituted isoquinolinol compounds having cardiotonic, phosphodiesterase fraction III inhibiting properties, and/or renal vasodilating properties

INVENTOR(S): Kanojia, Ramesh M.; Falotico, Robert; Tobia, Alfonso J.; Press, Jeffery B.

PATENT ASSIGNEE(S): Ortho Pharmaceutical Corp., USA

SOURCE: U.S., 11 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

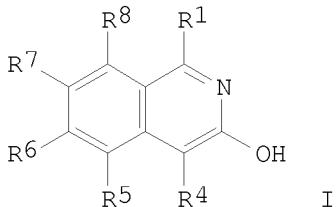
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4714705	A	19871222	US 1986-882655	19860707 <--
DK 8703480	A	19880108	DK 1987-3480	19870706 <--
FI 8702980	A	19880108	FI 1987-2980	19870706 <--
NO 8702812	A	19880108	NO 1987-2812	19870706 <--
AU 8775273	A	19880114	AU 1987-75273	19870706 <--
AU 597083	B2	19900524		
ZA 8704894	A	19890222	ZA 1987-4894	19870706 <--
IL 83088	A	19910816	IL 1987-83088	19870706 <--
EP 252721	A1	19880113	EP 1987-306002	19870707 <--
EP 252721	B1	19911002		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 63022562	A	19880130	JP 1987-167955	19870707 <--
CN 87105724	A	19880309	CN 1987-105724	19870707 <--
HU 44515	A2	19880328	HU 1987-3058	19870707 <--
HU 196966	B	19890228		
AT 67992	T	19911015	AT 1987-306002	19870707 <--
ES 2040750	T3	19931101	ES 1987-306002	19870707 <--
PRIORITY APPLN. INFO.:			US 1986-882655	A 19860707
			EP 1987-306002	A 19870707
OTHER SOURCE(S):	CASREACT 108:186593			

STN

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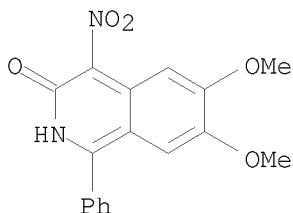
AB The title compds. I [R1 = H, (halo)alkyl, (halo)Ph, (halo)naphthyl; R4 = NO₂, NO, NH₂, di-C1-5-alkylamino, NHCO(Y)(R)_n; R = H, alkyl, C3-6 cycloalkyl, Ph, naphthyl, etc.; Y = O, N(H)x; R₅, R₆, R₇, R₈ = H, halo, HO, alkoxy; R₅R₆, R₆R₇, R₇R₈ = OCH₂O; x, n = 0-2] and their pharmaceutical salts, were prepared I (R1 = Me; R4 = NH₂; R6, R7 = MeO) as the diacetate solvate in AcOH at room temperature was reacted with Me(CH₂)₂CH₂NCO to give I (R1 = Me; R4 = BuNHCONH; R6, R7 = MeO) (III). III and other I each exhibited 1 or more of cardiotonic and renal vasodilating properties and phosphodiesterase fraction III inhibiting properties.

IT 113982-83-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as drug)

RN 113982-83-5 HCPLUS

CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-4-nitro-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 29 OF 29 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1984:174683 HCPLUS

DOCUMENT NUMBER: 100:174683

ORIGINAL REFERENCE NO.: 100:26565a,26568a

TITLE: 1-Phenylisoquinoline derivatives

INVENTOR(S): Konz, Elmar; Kruse, Hansjoerg; Hock, Franz

PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.

SOURCE: Ger. Offen., 24 pp.

STN

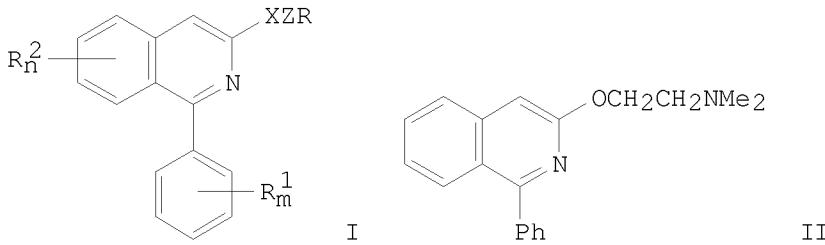
DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

CODEN: GWXXBX

Patent
German

1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3227741	A1	19840126	DE 1982-3227741 DE 1982-3227741	19820724 <-- 19820724
PRIORITY APPLN. INFO.:			CASREACT 100:174683; MARPAT 100:174683	
OTHER SOURCE(S): GI				



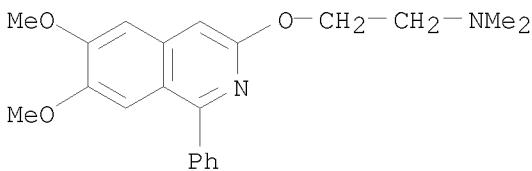
AB Title compds. (I) [X = O or S; m, n = 0-2; Z = bond or (un)substituted C1-8 alkylene; R = (un)substituted amino or N heterocyclyl; R₁ = H, halo, OH, NO₂, NH₂, C1-6 alkyl or alkoxy; R₂ = H, halo, OH, NH₂, NO₂, C1-6 alkyl or alkoxy, benzyloxy, OCH₂O, OCH₂CH₂O] were prepared and shown to have antidepressant activity. Thus, 6.6 g 1-phenyl-3-isoquinolinol, 2.16 g 50% NaH, and 150 mL PhMe were stirred 1 h at 60°, cooled to 20°, treated dropwise with 5.3 g Me₂NCH₂CH₂Cl, and stirred 2 h at 100° to give the isoquinolyl ether II.

IT 89707-24-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antidepressant)

RN 89707-24-4 HCPLUS

CN Ethanamine, 2-[(6,7-dimethoxy-1-phenyl-3-isoquinolinyloxy)-N,N-dimethyl-
(CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

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=> d his

(FILE 'HOME' ENTERED AT 19:20:54 ON 05 NOV 2009)

FILE 'REGISTRY' ENTERED AT 19:21:02 ON 05 NOV 2009

L1 STRUCTURE UPLOADED
L2 759 S 1L
L3 1677 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:24:12 ON 05 NOV 2009

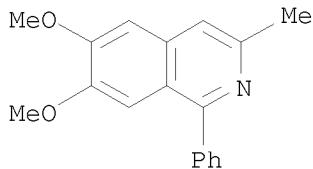
L4 376 S L3
L5 58 S L3/USES
L6 4 S L4 AND TROTTER, B?/AU
L7 372 S L4 NOT L6
L8 0 S L7 AND NANDA, K?/AU
L9 0 S L7 AND KETT, N?/AU
L10 0 S L7 AND DINSMORE, C?/AU
L11 0 S L7 AND PONTICELLO, G?/AU
L12 0 S L7 AND CLAREMON, D?/AU
L13 310 S L4 AND PD < OCTOBER 2003
L14 29 S L5 AND PD < OCTOBER 2003

=> d l13, ibib abs fhitstr, 1-310

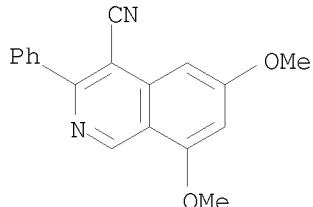
THE ESTIMATED COST FOR THIS REQUEST IS 1748.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L13 ANSWER 1 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1383638 HCAPLUS
DOCUMENT NUMBER: 149:575974
TITLE: The Beckmann reactions: rearrangements,
elimination-additions, fragmentations, and
rearrangement-cyclizations
AUTHOR(S): Gawley, Robert E.
CORPORATE SOURCE: University of Miami, Coral Gables, FL, USA
SOURCE: Organic Reactions (Hoboken, NJ, United States) (1988), 35, No pp. given
CODEN: ORHNBA
URL: <http://www3.interscience.wiley.com/cgi-bin/mrwhome/107610747/HOME>
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:575974
AB A review of the article The Beckmann reactions: rearrangements, elimination-addns., fragmentations, and rearrangement-cyclizations.
IT 20225-88-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(The Beckmann Reactions: Rearrangements, Elimination-Addns., Fragmentations, and Rearrangement-Cyclizations)
RN 20225-88-1 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-3-methyl-1-phenyl- (CA INDEX NAME)

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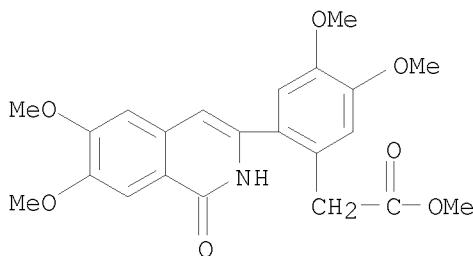
L13 ANSWER 2 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1383628 HCPLUS
DOCUMENT NUMBER: 149:555120
TITLE: The Vilsmeier reaction of non-aromatic compounds
AUTHOR(S): Jones, Gurnos; Stanforth, Stephen P.
CORPORATE SOURCE: University of Keele, Keele, UK
SOURCE: Organic Reactions (Hoboken, NJ, United States) (2000), 56, No pp. given
CODEN: ORHNBA
URL: <http://www3.interscience.wiley.com/cgi-bin/mrwhome/107610747/HOME>
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:555120
AB A review of the article The Vilsmeier reaction of non-aromatic compds.
IT 19713-14-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(The Vilsmeier Reaction of Non-Aromatic Compds.)
RN 19713-14-5 HCPLUS
CN 4-Isoquinolinecarbonitrile, 6,8-dimethoxy-3-phenyl- (CA INDEX NAME)



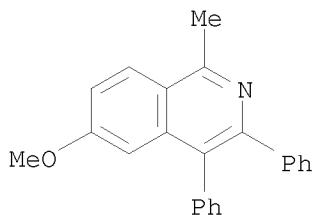
L13 ANSWER 3 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1383571 HCPLUS
DOCUMENT NUMBER: 149:555084
TITLE: Aromatic substitution by the SRN1 reaction
AUTHOR(S): Rossi, Roberto A.; Pierini, Adriana B.; Santiago, Ana N.
CORPORATE SOURCE: Universidad Nacional de Cordoba, Cordoba, Argent.
SOURCE: Organic Reactions (Hoboken, NJ, United States) (1999), 54, No pp. given
CODEN: ORHNBA
URL: <http://www3.interscience.wiley.com/cgi-bin/mrwhome/107610747/HOME>
PUBLISHER: John Wiley & Sons, Inc.

STN

DOCUMENT TYPE: Journal; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:555084
AB A review of the article Aromatic substitution by the SRN1 reaction.
IT 144709-22-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(A review of the article Aromatic substitution by the SRN1 reaction)
RN 144709-22-8 HCAPLUS
CN Benzeneacetic acid, 2-(1,2-dihydro-6,7-dimethoxy-1-oxo-3-isooquinolinyl)-
4,5-dimethoxy-, methyl ester (CA INDEX NAME)

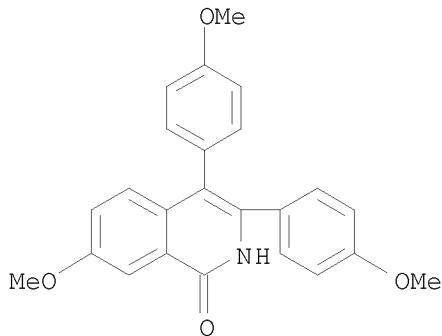


L13 ANSWER 4 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:994686 HCAPLUS
DOCUMENT NUMBER: 149:307083
TITLE: Chlorotris(triphenylphosphine)-rhodium(I)
AUTHOR(S): Burgess, Kevin; van der Donk, Wilfred A.
CORPORATE SOURCE: USA
SOURCE: e-EROS Encyclopedia of Reagents for Organic Synthesis
(2001), No pp. given. John Wiley & Sons,
Ltd.: Chichester, UK.
CODEN: 69KUHI
URL: <http://www3.interscience.wiley.com/cgi-bin/mrwhome/104554785/HOME>
DOCUMENT TYPE: Conference; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:307083
AB A review of the article Chlorotris(triphenylphosphine)-rhodium(I).
IT 585531-20-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Chlorotris(triphenylphosphine)-rhodium(I))
RN 585531-20-0 HCAPLUS
CN Isoquinoline, 6-methoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)



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L13 ANSWER 5 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:994122 HCPLUS
DOCUMENT NUMBER: 149:306545
TITLE: Isocyanic Acid
AUTHOR(S): Narula, Acharan S.; Ramachandran, Kishore
CORPORATE SOURCE: USA
SOURCE: e-EROS Encyclopedia of Reagents for Organic Synthesis (2001), No pp. given. John Wiley & Sons, Ltd.: Chichester, UK.
CODEN: 69KUHI
URL: <http://www3.interscience.wiley.com/cgi-bin/mrwhome/104554785/HOME>
DOCUMENT TYPE: Conference; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:306545
AB A review of the article Isocyanic Acid.
IT 93119-93-8P
RL: SPN (Synthetic preparation); PREP (Preparation) (Isocyanic Acid)
RN 93119-93-8 HCPLUS
CN 1(2H)-Isoquinolinone, 7-methoxy-3,4-bis(4-methoxyphenyl)- (CA INDEX NAME)



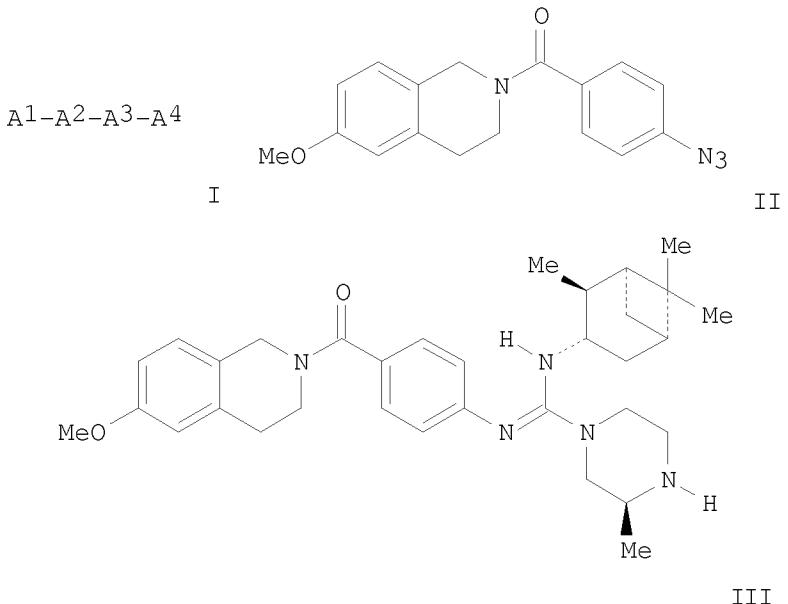
L13 ANSWER 6 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:497495 HCPLUS
DOCUMENT NUMBER: 143:43783
TITLE: Preparation of (guanidinophenyl)isoquinolines and related compounds as MC4-R agonists
INVENTOR(S): Boyce, Rustum; Chu, Daniel
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 351,574.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US	20050124652	A1	20050609	US	2005-503392	20050126
US	20030195187	A1	20031016	US	2003-351574	20030127
WO	2003066597	A2	20030814	WO	2003-US1078	20030203 <--
WO	2003066597	A3	20040401			
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
RITY APPLN. INFO.:			US 2002-353188P	P	20020204	
			US 2003-351574	A2	20030127	
			WO 2003-US1078	W	20030203	

OTHER SOURCE(S): CASREACT 143:43783; MARPAT 143:43783

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AB Title compds. I [A1 = NR4C(=NR3)NR1R2, N=C(NR3R4)(NR1R2); R1 = H, (un)substituted alkyl, alkenyl, etc.; R2 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R3 = (un)substituted aryl, alkyl, alkenyl, etc.; R4 = H, (un)substituted alkyl, alkenyl, etc.; A2 = (un)substituted aryl, heteroaryl; A3 = covalent bond, linking group, e.g., O, S, CO, etc.; A4 = (un)substituted arylalkyl, heteroarylalkyl, aryl, etc.] and their pharmaceutically acceptable salts were prepared. For example, trimethylphosphine mediated reduction of phenylazide II followed by the sequential addition of (1S,2S,3S,5S)-2,6,6-trimethylbicyclo[3.1.1]heptan-3-

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isocyanate and (S)-(+)-2-methylpiperazine, afforded (guanidinophenyl)isoquinoline III. Compds. I are claimed to be useful for the treatment of obesity and type II diabetes.

IT 581101-76-0P

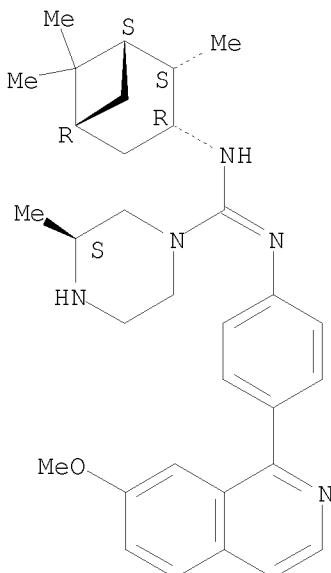
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (guanidinophenyl)isoquinolines and related compds. as MC4-R agonists)

RN 581101-76-0 HCPLUS

CN 1-Piperazinecarboximidamide, N-[4-(7-methoxy-1-isoquinolinyl)phenyl]-3-methyl-N'-(1S,2S,3R,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl]-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 7 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:69041 HCPLUS

DOCUMENT NUMBER: 140:253507

TITLE: On triazoles. XLIX. Synthesis of 5,6-dihydrothiazolo[3,2-b][1,2,4]triazol-2-yl-, 6,7-dihydro-5H-[1,2,4]triazolo[5,1-b][1,3]thiazin-2-yl-, and 5,6,7,8-tetrahydro[1,2,4]triazolo[5,1-b][1,3]thiazepin-2-ylisoquinolinium salts

AUTHOR(S): Prauda, Ibolya; Reiter, Jozsef

CORPORATE SOURCE: Egis Pharmaceuticals Ltd., Budapest, H-1475, Hung.

SOURCE: Journal of Heterocyclic Chemistry (2003),

40(6), 1041-1050

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

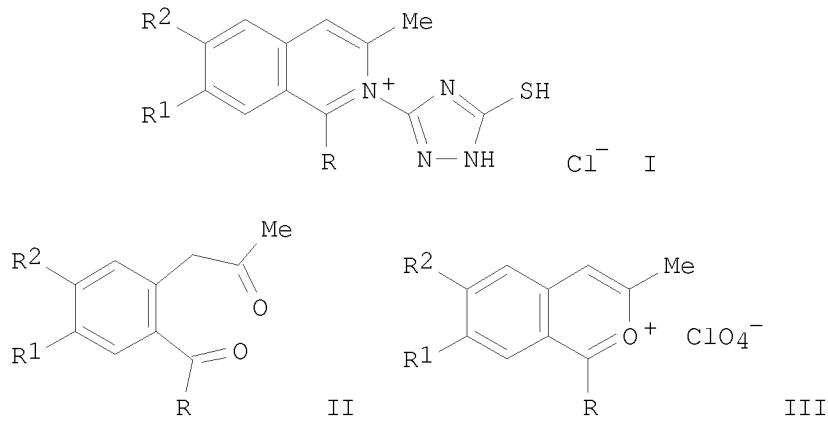
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:253507

STN

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AB 5'-Mercapto-1'H-1,2,4-triazol-3'-ylisoquinolinium salts (I, R = Pr, 4-FC₆H₄, etc.; R¹R² = OCH₂O; R¹ = R² = MeO) were synthesized by the reaction of ortho-acyl phenylacetones (II) or the corresponding pyrylium salts (III) and 5-amino-2,3-dihydro-1H-1,2,4-triazole-3-thione. Treatment of thiopholes I with α,ω -dibromoalkanes led to isoquinolinium salts condensed with thiazole, thiazine and thiazepine rings. When I are reacted with dibromomethane, type dimeric structures are obtained.

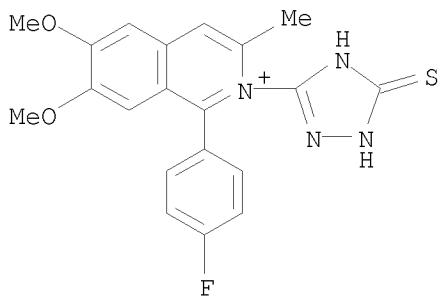
IT 670225-13-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 5,6-dihydrothiazolo[3,2-b][1,2,4]triazol-2-yl-, 6,7-dihydro-5H-[1,2,4]triazolo[5,1-b][1,3]thiazin-2-yl-, and 5,6,7,8-tetrahydro[1,2,4]triazolo[5,1-b][1,3]thiazepin-2-ylisoquinolinium salts)

RN 670225-13-5 HCAPLUS

CN Isoquinolinium, 2-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-1-(4-fluorophenyl)-6,7-dimethoxy-3-methyl-, chloride (1:1) (CA INDEX NAME)



● Cl⁻

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:941009 HCAPLUS
DOCUMENT NUMBER: 140:280814
TITLE: Effects of topoisomerases inhibitors protoberberine on Leishmania donovani growth, macrophage function, and infection
AUTHOR(S): Marquis, Jean-Francois; Makhey, Darshan; LaVoie, Edmond J.; Olivier, Martin
CORPORATE SOURCE: Departement de Biologie Medicale, Faculte de Medecine, Centre de Recherche en Infectiologie du CHUQ, Universite Laval, Sainte-Foy, QC, G1V 4G2, Can.
SOURCE: Journal of Parasitology (2003), 89(5), 1048-1052
CODEN: JOPAA2; ISSN: 0022-3395
PUBLISHER: American Society of Parasitologists
DOCUMENT TYPE: Journal
LANGUAGE: English
AB DNA topoisomerases play a pivotal role in the regulation of cell division. Inhibition of Leishmania spp. topoisomerases represents an alternative to control parasite growth. Cancer research led to the development of several potent topoisomerase inhibitors such as topoisomerase 1, topoisomerase 17, or both (monobenzimidazole, terbenzimidazole, and protoberberine alkaloid-related compds.) that are effective antitumor agents. In the present study, we evaluated the efficacy of these compds. against Leishmania spp. growth in vitro. Some protoberberine compds. showed pronounced antileishmanial activity and were selected for further anal. in macrophages. These compds. did not affect macrophage viability and only slightly reduced macrophage nitric oxide generation in response to interferon- γ . Moreover, exposure of infected macrophages to these compds. significantly reduced parasite loads. Collectively, our data suggest that protoberberine-related compds. have powerful antileishmania action and that minor structural variations among them can substantially improve their activity to restrict Leishmania spp. infection in vitro.

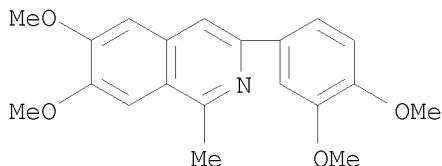
STN

IT 35989-93-6

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(topoisomerase inhibitors protoberberine derivs. effects on Leishmania donovani growth, macrophage function, and infection)

RN 35989-93-6 HCAPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 9 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:906475 HCAPLUS

DOCUMENT NUMBER: 140:106853

TITLE: Predicting the Genotoxicity of Polycyclic Aromatic Compounds from Molecular Structure with Different Classifiers

AUTHOR(S): He, Linnan; Jurs, Peter C.; Custer, Laura L.; Durham, Stephen K.; Pearl, Greg M.

CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA

SOURCE: Chemical Research in Toxicology (2003), 16(12), 1567-1580

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

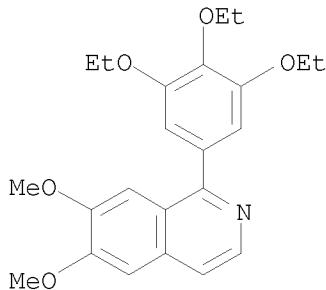
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Classification models were developed to provide accurate prediction of genotoxicity of 277 polycyclic aromatic compds. (PACs) directly from their mol. structures. Numerical descriptors encoding the topol., geometric, electronic, and polar surface area properties of the compds. were calculated to represent the structural information. Each compound's genotoxicity was represented with IMAX (maximal SOS induction factor) values measured by the SOS Chromotest in the presence and absence of S9 rat liver homogenate. The compds.' class identity was determined by a cutoff IMAX value of 1.25-compds. with IMAX > 1.25 in either test were classified as genotoxic, and the ones with IMAX ≤ 1.25 were nongenotoxic. Several binary classification models were generated to predict genotoxicity: k-nearest neighbor (k-NN), linear discriminant anal., and probabilistic neural network. The study showed k-NN to provide the highest predictive ability among the three classifiers with a training set classification rate of 93.5%. A consensus model was also developed that incorporated the three classifiers and correctly predicted 81.2% of the 277 compds. It also provided a higher prediction rate on the genotoxic class than any other

STN

single model.
IT 549-68-8, Octaverine
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL
(Biological study)
(predicting genotoxicity of polycyclic aromatic compds. from mol.
structure with different classifiers)
RN 549-68-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS
RECORD (24 CITINGS)
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

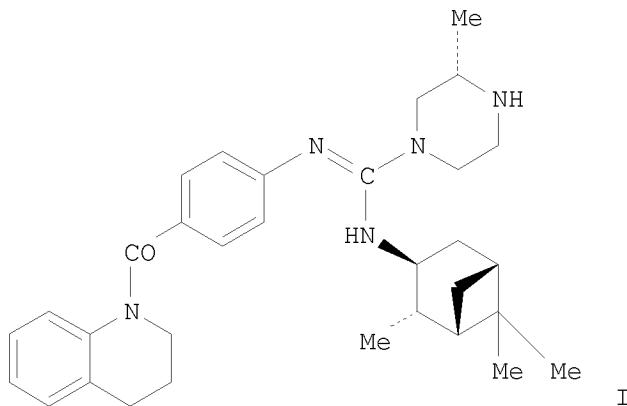
L13 ANSWER 10 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:633668 HCPLUS
DOCUMENT NUMBER: 139:197505
TITLE: Preparation of aryl- or heteroaryl-containing
guanidines as melanocortin-4-receptor agonists useful
against disorders such as obesity or type II diabetes
INVENTOR(S): Boyce, Rustum; Chu, Daniel
PATENT ASSIGNEE(S): Chiron Corporation, USA
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003066597	A2	20030814	WO 2003-US1078	20030203 <--
WO 2003066597	A3	20040401		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

US 20030195187	A1	20031016	US 2003-351574	20030127
AU 2003216053	A1	20030902	AU 2003-216053	20030203 <--
EP 1478626	A2	20041124	EP 2003-737536	20030203
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006503799	T	20060202	JP 2003-565971	20030203
US 20050124652	A1	20050609	US 2005-503392	20050126
PRIORITY APPLN. INFO.:				
			US 2002-353188P	P 20020204
			US 2003-351574	A 20030127
			WO 2003-US1078	W 20030203

OTHER SOURCE(S): MARPAT 139:197505

GI



AB A variety of small, guanidino group-containing mols. (I; A1-A2-A3-A4; variables defined below; e.g. (3S)-N'-(4-(3,4-dihydroquinolin-1(2H)-ylcarbonyl)phenyl)-3-methyl-N-[(1S,2S,3S,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl]piperazine-1-carboximidamide (shown as I)) capable of acting as MC4-R agonists are provided. The compds. are useful in treating MC4-R mediated diseases and may be formulated into pharmaceutical formulations and compns. Although the methods of preparation are not claimed, several example preps. of I and a number of example preps. of intermediates are included; 131 addnl. examples of I are tabulated with mass spectral characterization data. Some of the I have -log EC50 values above .apprx.3. Compds. I showed beneficial effects in in vivo studies on energy intake, body weight, hyperinsulinemia, and glucose levels in male 9-10 wk old ob/ob mice that display early onset of obesity, insulin resistance and diabetes due to leptin deficiency. For I: A1 = R1'R2'NC(:NR3')NR4'-, R1'R2'NC(NR3'R4'):N-; R1' = H, and (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, heterocyclyl, arylalkyl, heteroarylalkyl, and cycloalkylalkyl; R2' = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, heterocyclyl, arylalkyl, heteroarylalkyl, and cycloalkylalkyl; or R1' and R2', together with the N to which they are bound, form a (un)substituted heterocyclyl or heteroaryl; R3' = (un)substituted aryl, alkyl, alkenyl, alkynyl, cycloalkyl, heteroaryl, heterocyclyl, heterocyclylalkyl, arylalkyl, heteroarylalkyl, and cycloalkylalkyl; R4' = H, and (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, heterocyclylalkyl, cycloalkylalkyl, aryl, heteroaryl, heterocyclyl, arylalkyl, and heteroarylalkyl. A2 =

(un)substituted aryl and heteroaryl; A3 is a covalent bond such that A2 is directly bonded to A4, or A3 is a linking group O, S, -NRa-, -C(O)-, -C(O)O-, -NRaC(O)-, -SO2NRa-, -C(S)-, -C(O)S-, -P(O)Rb-, -SO2-, and -S(O)-, wherein if A3 is a linking group, then it is bonded to A2 and A4 in a configuration A2-O-A4, A2-S-A4, A2-NRa-A4, A2-C(O)-A4, A2-C(O)O-A4, A4-C(O)O-A2, A2-NRaC(O)-A4, A4-NRaC(O)-A2, A2-SO2NRa-A4, A4-SO2NRa-A2, A2-C(S)-A4, A2-(C:O)S-A4, A4-(C:O)S-A2, A2-(P:O)Rb-A4, A2-SO2-A4, and A2-S(O)-A4 provided that if A3 is a linking group with the configuration A4-NRaC(O)-A2, then A2 is not a (un)substituted Ph and is not a (un)substituted 6-membered N-containing heteroaryl. A4 = (un)substituted arylalkyl, heteroarylalkyl, aryl, heteroaryl, heterocyclyl, cycloalkyl, heterocyclylalkyl, cycloalkylalkyl, alkenyl, alkynyl, and alkyl; Ra = H, and (un)substituted arylalkyl, heteroarylalkyl, aryl, heteroaryl, heterocyclyl, cycloalkyl, heterocyclylalkyl, cycloalkylalkyl, alkenyl, alkynyl, and alkyl; Rb = (un)substituted arylalkyl, heteroarylalkyl, aryl, heteroaryl, heterocyclyl, cycloalkyl, heterocyclylalkyl, cycloalkylalkyl, alkenyl, alkynyl, and alkyl.

IT 581101-76-0P, (3S)-3-Methyl-N-[4-[7-(methyloxy)isoquinolin-1-yl]phenyl]-N'-(1S,2S,3R,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl)piperazine-1-carboximidamide

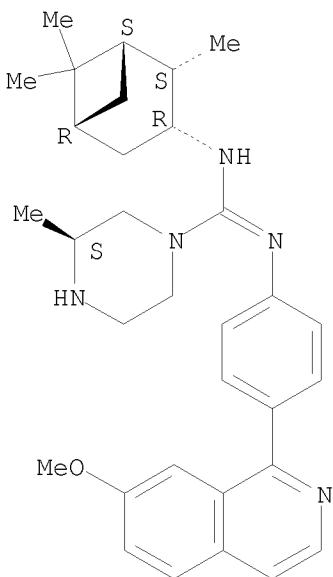
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of aryl- or heteroaryl-containing guanidines as melanocortin-4-receptor agonists useful against disorders such as obesity or type II diabetes)

RN 581101-76-0 HCPLUS

CN 1-Piperazinecarboximidamide, N-[4-(7-methoxy-1-isoquinolinyl)phenyl]-3-methyl-N'-(1S,2S,3R,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl-, (3S)-(CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT:

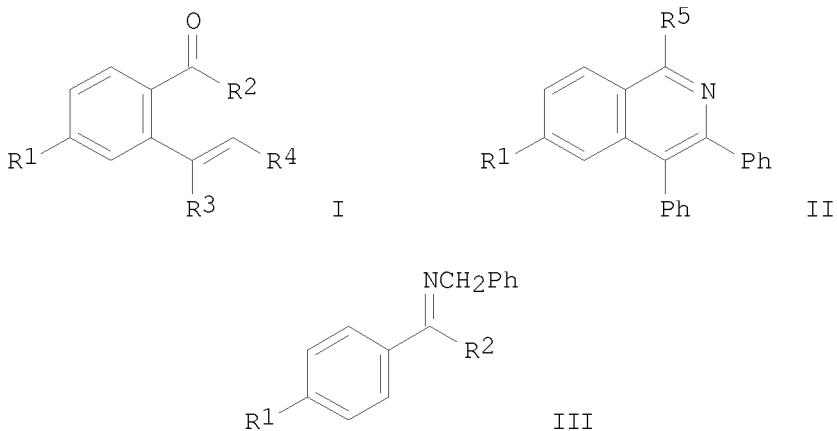
5

THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD

(5 CITINGS)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 11 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:505035 HCAPLUS
 DOCUMENT NUMBER: 139:197350
 TITLE: Rh(I)-Catalyzed Direct ortho-Alkenylation of Aromatic Ketimines with Alkynes and its Application to the Synthesis of Isoquinoline Derivatives
 AUTHOR(S): Lim, Sung-Gon; Lee, Jun Hee; Moon, Choong Woon; Hong, Jun-Bae; Jun, Chul-Ho
 CORPORATE SOURCE: Department of Chemistry, Yonsei University, Seoul, 120-749, S. Korea
 SOURCE: Organic Letters (2003), 5(15), 2759-2761
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:197350
 GI



AB Novel synthetic methods for preparation of both ortho-alkenylated aromatic ketones

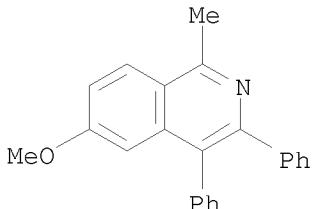
I ($R_1 = H, F^3C, MeO$; $R_2 = Me, Et, n\text{-pentyl}$; $R_3 = H, R_4 = Bu, Me^3C, n\text{-hexyl}$; $R_3 = R_4 = Ph$) and isoquinolines II ($R_5 = Me, PhCH_2CH_2$) have been developed via the Rh(I)-catalyzed direct ortho-alkenylation of common aromatic ketimines III with alkynes $R_3C\text{.tptbond.CR}_4$. Furthermore, a highly efficient one-pot synthesis of isoquinolines II was achieved by simply mixing aromatic ketone $4-R_1C_6H_4COMe$, benzylamine, and diphenylacetylene in the presence of a Rh(I) catalyst.

IT 585531-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of alkenylphenyl ketones, alkenylphenyl ketimines and isoquinolines via Rh(I)-catalyzed direct ortho-alkenylation of aromatic

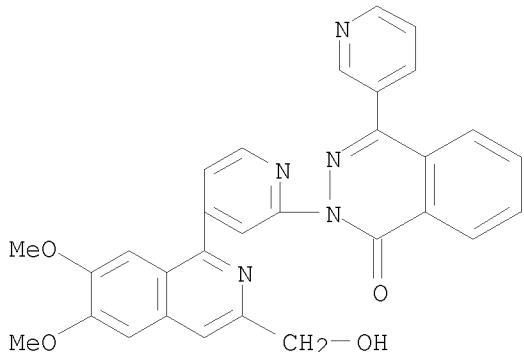
STN

 ketimines with alkynes)
RN 585531-20-0 HCAPLUS
CN Isoquinoline, 6-methoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 36 THERE ARE 36 CAPLUS RECORDS THAT CITE THIS
REFERENCE COUNT: 20 RECORD (36 CITINGS)
 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 12 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:485887 HCAPLUS
DOCUMENT NUMBER: 139:261143
TITLE: Synthesis and biological activities of
 1-pyridylisoquinoline and 1-pyridyldihydroisoquinoline
 derivatives as PDE4 inhibitors
AUTHOR(S): Ukita, Tatsuzo; Sugahara, Masakatsu; Terakawa,
 Yoshihiro; Kuroda, Tooru; Wada, Kazuteru; Nakata, Aya;
 Kikkawa, Hideo; Ikezawa, Katsuo; Naito, Kazuaki
CORPORATE SOURCE: Discovery Research Laboratory, Tanabe Seiyaku Co.,
 Ltd., 3-16-89, Kashima, Yodogawa, Osaka, 532-8505,
 Japan
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003
), 13(14), 2347-2350
 CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:261143
AB A novel series of 1-pyridylisoquinoline and 1-pyridyldihydroisoquinoline
derivs. has been prepared. These compds. showed potent PDE4 inhibitory
activities and a broad margin between the Ki value of the rolipram binding
affinity and the IC50 value of PDE4 inhibition. They also exhibited
potent inhibitory activities toward LPS-induced TNF- α production in
mice.
IT 209261-39-2P
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
 SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and biol. activities of pyridylisoquinoline and
 pyridyldihydroisoquinoline derivs. as PDE4 inhibitors)
RN 209261-39-2 HCAPLUS
CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-
 isoquinolinyl]-2-pyridinyl]-4-(3-pyridinyl)-, hydrochloride (1:1) (CA
 INDEX NAME)



● HCl

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 13 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:463808 HCPLUS
DOCUMENT NUMBER: 139:173185
TITLE: Synthesis and Structure-Activity Studies of Novel
Orally Active Non-Terpenoic 2,3-Oxidosqualene Cyclase
Inhibitors
AUTHOR(S): Dehmlow, Henrietta; Aebi, Johannes D.; Jolidon,
Synese; Ji, Yu-Hua; Von Mark, Elisabeth M.; Himber,
Jacques; Morand, Olivier H.
CORPORATE SOURCE: Pharmaceuticals Division, Preclinical Research, F.
Hoffmann-La Roche Ltd., Basel, CH-4070, Switz.
SOURCE: Journal of Medicinal Chemistry (2003),
46(15), 3354-3370
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:173185
AB New orally active non-terpenoic inhibitors of human 2,3-oxidosqualene cyclase (hOSC) are reported. The starting point for the optimization process was a set of compds. derived from a fungicide project, which in addition to showing high affinity for OSC from *Candida albicans* showed also high affinity for human OSC. Common structural elements of these inhibitors are an amine residue and an electrophilic carbonyl C atom embedded in a benzophenone system, which are at a distance of about 10.7 Å. Considering that the keto moiety is in a potentially labile position, modifications of the substitution pattern at the benzophenone as well as annelated heteroaryl systems were explored. Our approach combined testing of the compds. first for increased binding affinity and for increased stability *in vitro*. Most promising compds. were then evaluated for their efficacy in lowering plasma total cholesterol (TC) and plasma low-d. lipoprotein cholesterol (LDL-C) in hyperlipidemic hamsters. In

STN

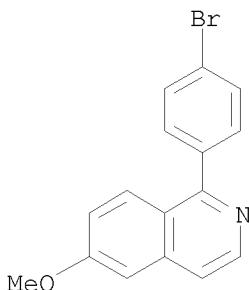
this respect, the most promising compds. are the benzophenone derivative 1-fumarate and the benzo[d]isothiazol 24-fumarate, which lowered TC by 40% and 33%, resp.

IT 579815-94-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and structure-activity studies of non-terpenoic
oxidosqualene cyclase inhibitors)

RN 579815-94-4 HCPLUS

CN Isoquinoline, 1-(4-bromophenyl)-6-methoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 14 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:311225 HCPLUS

DOCUMENT NUMBER: 139:270245

TITLE: Structure-based approach to falcipain-2 inhibitors:
synthesis and biological evaluation of
1,6,7-Trisubstituted dihydroisoquinolines and
isoquinolines

AUTHOR(S): Batra, Sanjay; Sabnis, Yogesh A.; Rosenthal, Philip J.; Avery, Mitchell A.

CORPORATE SOURCE: Medicinal Chemistry Division, Central Drug Research Institute, Lucknow, 226001, India

SOURCE: Bioorganic & Medicinal Chemistry (2003),
11(10), 2293-2299

PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:270245

AB 1,4,7-Trisubstituted isoquinolines were designed, synthesized and evaluated for their inhibition against Plasmodium falciparum cysteine protease falcipain-2. The 1-benzylxyphenyl-dihydroisoquinoline and -isoquinoline derivs. were found to exhibit better activity against falcipain-2 than their corresponding 1-hydroxyphenyl or 1-methoxyphenyl analogs. The docking scores correlate with the IC50 values of compds. and give a high coefficient correlation of 0.94.

IT 605657-60-1P

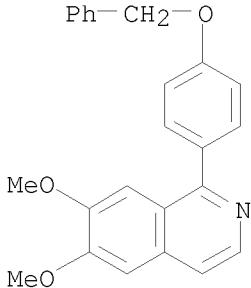
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

STN

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis, antimalarial effect and structure-activity relationship of dihydroisoquinoline and isoquinoline derivs. as falcipain-2 inhibitors)

RN 605657-60-1 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-[4-(phenylmethoxy)phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 27 THERE ARE 27 CAPLUS RECORDS THAT CITE THIS RECORD (27 CITINGS)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 15 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:282400 HCPLUS
DOCUMENT NUMBER: 138:309280
TITLE: Combinations containing a phosphodiesterase inhibitor
INVENTOR(S): Cohen, David Saul
PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis-Erfindungen Verwaltungsgesellschaft M.B.H.; Novartis Pharma GmbH
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003028730	A2	20030410	WO 2002-EP10826	20020926 <--
WO 2003028730	A3	20030904		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR				
US 20030114469	A1	20030619	US 2002-231427	20020828 <--
US 20030139429	A1	20030724	US 2002-236651	20020906 <--
US 7019010	B2	20060328		
CA 2458343	A1	20030410	CA 2002-2458343	20020926 <--
AU 20022338806	A1	20030414	AU 2002-338806	20020926 <--
EP 1432423	A2	20040630	EP 2002-777227	20020926

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
 BR 2002012852 A 20041013 BR 2002-12852 20020926
 JP 2005504113 T 20050210 JP 2003-532062 20020926
 CN 1694707 A 20051109 CN 2002-819046 20020926
 US 20060106039 A1 20060518 US 2006-324999 20060103
 PRIORITY APPLN. INFO.: US 2001-325485P P 20010927
 US 2002-231427 B2 20020828
 US 2002-236651 A3 20020906
 WO 2002-EP10826 W 20020926

OTHER SOURCE(S): MARPAT 138:309280

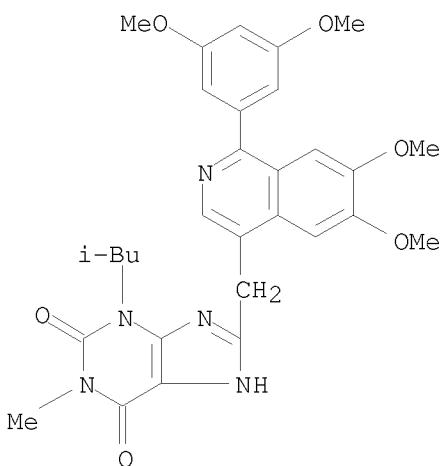
AB The present invention relates to a pharmaceutical composition, comprising (a) a phosphodiesterase 5 inhibitor or a pharmaceutically acceptable salt thereof and (b) at least one of the active ingredients selected from the group consisting of (i) an anti-diabetic agent; (ii) HMG-Co-A reductase inhibitors; (iii) an antihypertensive agent; and (iv) a serotonin reuptake inhibitor (SSRI) or, in each case, or a pharmaceutically acceptable salt thereof and a pharmaceutically acceptable carrier. The pharmaceutical composition may be employed for the treatment of sexual dysfunction, hyperglycemia, hyperinsulinemia, hyperlipidemia, hypertriglyceridemia, diabetes, insulin resistance, impaired glucose metabolism, conditions of impaired glucose tolerance (IGT), conditions of impaired fasting plasma glucose, obesity, diabetic retinopathy, diabetic nephropathy, glomerulosclerosis, diabetic neuropathy, syndrome X, erectile dysfunction, coronary heart disease, hypertension, especially ISH, angina pectoris, myocardial infarction, stroke, vascular restenosis, endothelial dysfunction, impaired vascular compliance, congestive heart failure.

IT 366444-39-5

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (compns. containing PDE5 inhibitor in combination with antidiabetic, HMG-Co-A reductase inhibitor, antihypertensive, or serotonin reuptake inhibitor)

RN 366444-39-5 HCPLUS

CN 1H-Purine-2,6-dione, 8-[(1-(3,5-dimethoxyphenyl)-6,7-dimethoxy-4-isoquinolinyl)methyl]-3,9-dihydro-1-methyl-3-(2-methylpropyl)-(CA INDEX NAME)



STN

OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(16 CITINGS)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 16 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:188741 HCPLUS
DOCUMENT NUMBER: 138:303768
TITLE: Electronic spectra and crystal structure of
1-methyl-3-phenyl-6,7 dimethoxyisoquinoline
AUTHOR(S): Kakas, Marija I.; Janic, Ivan G.; Kapor, Agnes J.;
Willett, Roger D.; Simon, Lajos L.; Bernath, Gabor G.
CORPORATE SOURCE: Institute of Physics, Faculty of Natural Sciences,
University of Novi Sad, Novi Sad, YU-21000, Yugoslavia
SOURCE: Zbornik Matice Srpske za Prirodne Nauke (2002
, Volume Date 2001, 101, 25-35
CODEN: ZMSNEI; ISSN: 0352-4906

PUBLISHER: Matica Srpska

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1-Methyl-3-phenyl-6,7-dimethoxyisoquinoline has been prepared by Pictet-Gams reaction in order to prove its real structure i.e. to exclude the possibility of aryl migration found by Bindra et al. (1968) in the case of the cyclization of some isoquinolines. In order to achieve a better understanding of the mol.'s features and to establish the possible migration of the aryl group, we have performed a study of its crystal structure by x-ray diffraction method and correlated it with absorption (at 293 K), excitation and luminescence spectra of compound in solution and fluorescence spectra in microcryst. state at 293 and 77 K. Based on the absorption spectra it could be concluded that the Ph substituent was bonded to position 3. The anal. of emission and excitation spectra in the solution and emission spectra in the microcryst. state attested of large planarity of the mol. in the solid solution and crystalline environment. The great similarity of the spectra in the n-hexane solid solution and microcryst. state led to the conclusion that no strong intermol. interactions existed in the crystalline state. The x-ray anal. verified the formation of the desired and not of the aryl-migrated structure. The anal. of the mol. packing indicated that the planar mols. joined into pairs probably due to charge transfer. The layers formed by the pairs interacted only through van der Waals contacts.

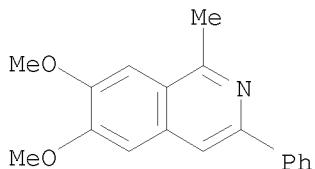
IT 52947-33-8, Isoquinoline, 6,7-dimethoxy-1-methyl-3-phenyl-

RL: PRP (Properties)

(crystal structure; electronic spectra and crystal structure of
1-methyl-3-phenyl-6,7 dimethoxyisoquinoline)

RN 52947-33-8 HCPLUS

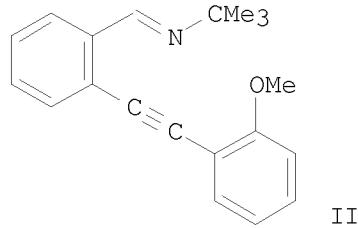
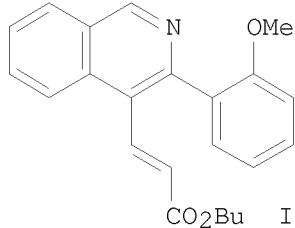
CN Isoquinoline, 6,7-dimethoxy-1-methyl-3-phenyl- (CA INDEX NAME)



STN

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 17 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:962175 HCPLUS
DOCUMENT NUMBER: 138:187626
TITLE: Synthesis of 4-(1-Alkenyl)isoquinolines by Palladium(II)-Catalyzed Cyclization/Olefination
AUTHOR(S): Huang, Qinhua; Larock, Richard C.
CORPORATE SOURCE: Department of Chemistry, Iowa State University, Ames, IA, 50011, USA
SOURCE: Journal of Organic Chemistry (2003), 68(3), 980-988
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187626
GI



AB 4-(1-Alkenyl)-3-arylisouinolines such as I are prepared in 20-97% yields by coupling of 2-(1-alkynyl)arylaldimines such as II with alkenes such as acrylates, vinyl sulfones, and styrene followed by cyclization in the presence of palladium (II) bromide, either copper (II) acetate or copper (II) chloride, and inorg. bases such as sodium acetate or sodium bicarbonate in DMSO. The reaction can be run either using copper (II) acetate as the stoichiometric oxidant with sodium acetate as the base or using copper (II) chloride as an oxidation catalyst with oxygen as the terminal oxidant and sodium bicarbonate as the base. An o-methoxyphenylalkynyl arylaldimines undergoes cyclocondensation to provide the corresponding isoquinolines in improved yields; the o-methoxy group facilitates the cyclocondensation by promoting the Pd-catalyzed cyclization and stabilizing the resulting Pd(II) intermediate. When secondary allylic alcs. are used as alkenes in the cyclocondensation reaction, saturated ketones are obtained as products.

IT 438565-07-2P

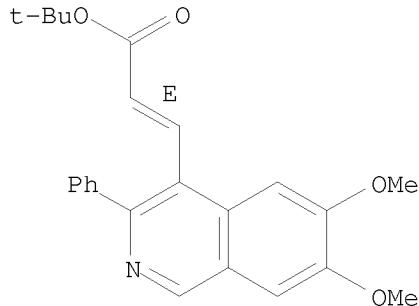
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (alkenyl)arylisouinolines by the one-step cyclization and stereoselective coupling reactions of (alkynyl) arylaldimines with alkenes in the presence of palladium and copper catalysts)

RN 438565-07-2 HCPLUS

CN 2-Propenoic acid, 3-(6,7-dimethoxy-3-phenyl-4-isouinolinyl)-, 1,1-dimethylethyl ester, (2E)- (CA INDEX NAME)

STN

Double bond geometry as shown.



OS.CITING REF COUNT: 63 THERE ARE 63 CAPLUS RECORDS THAT CITE THIS RECORD (63 CITINGS)
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 18 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:905931 HCAPLUS
DOCUMENT NUMBER: 137:389204
TITLE: Compositions for promoting healing of bone fracture containing phosphodiesterase 4 inhibitors
INVENTOR(S): Sakurai, Naoki; Takagi, Toshiki; Yanaka, Noriyuki; Horikiri, Yuji; Tamura, Takashi
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002094321	A1	20021128	WO 2002-JP4931	20020522 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2447619	A1	20021128	CA 2002-2447619	20020522 <--
AU 2002308878	A1	20021203	AU 2002-308878	20020522 <--
EP 1389468	A1	20040218	EP 2002-771772	20020522
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1520313	A	20040811	CN 2002-812733	20020522
MX 2003010679	A	20040302	MX 2003-10679	20031121
US 20040146561	A1	20040729	US 2003-478709	20031124
US 20080031958	A1	20080207	US 2007-826921	20070719

STN

PRIORITY APPLN. INFO.: JP 2001-154064 A 20010523
WO 2002-JP4931 W 20020522
US 2003-478709 A3 20031124

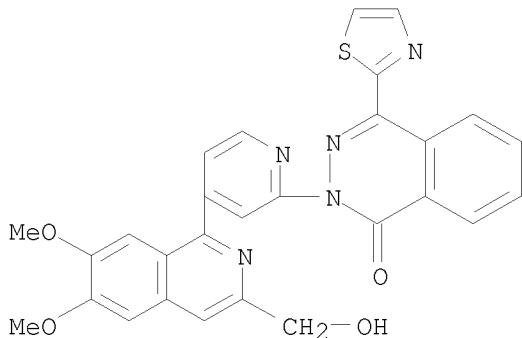
AB Disclosed are compns. for promoting healing of bone fracture which contain as the active ingredient a phosphodiesterase (PDE) 4 inhibitor having an effect of inhibiting PDE4, e.g. 2,3-bis(hydroxymethyl)-6,7-diethoxy-1-[1-(2-methoxyethyl)-2-oxo-4-pyridyl]-naphthalene and 2,3-bis(hydroxymethyl)-6,7-diethoxy-1-[2-(4-(3-pyridyl)-1(2H)-phthalazinone-2-yl)-4-pyridyl]-naphthalene, etc.. In particular, medicinal compns. containing the PDE4 inhibitor and a biocompatible and biodegradable polymer which exert an excellent effect of promoting quick healing of bone fracture when processed into dosage forms adequate for topical administration to bone fracture sites, for example, microspherical preps. These compns. are useful in treating bone fracture in, for example, aged persons, patients with diabetics and patients with osteoporosis which can be hardly repaired.

IT 209261-43-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. for promoting healing of bone fracture containing phosphodiesterase 4 inhibitors)

RN 209261-43-8 HCPLUS

CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-isoquinolinyl]-2-pyridinyl]-4-(2-thiazolyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 19 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:905929 HCPLUS

DOCUMENT NUMBER: 137:389203

TITLE: Therapeutic compositions for repairing chondropathy containing phosphodiesterase 4 inhibitors

INVENTOR(S): Takigawa, Masaharu; Sakurai, Naoki; Takagi, Toshiki; Yanaka, Noriyuki; Horikiri, Yuji; Tamura, Takashi

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 66 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

STN

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002094320	A1	20021128	WO 2002-JP4930	20020522 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2447618	A1	20021128	CA 2002-2447618	20020522 <--
AU 2002308877	A1	20021203	AU 2002-308877	20020522 <--
EP 1389467	A1	20040218	EP 2002-771771	20020522
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1537018	A	20041013	CN 2002-812647	20020522
MX 2003010672	A	20040302	MX 2003-10672	20031121
US 20040180900	A1	20040916	US 2003-478432	20031121
US 20070155652	A1	20070705	US 2007-707008	20070216
PRIORITY APPLN. INFO.:			JP 2001-154048	A 20010523
			WO 2002-JP4930	W 20020522
			US 2003-478432	A3 20031121

AB Therapeutic compns. for repairing chondropathy which contain as the active ingredient a phosphodiesterase (PDE) 4 inhibitor having an effect of inhibiting PDE4, e.g. 2,3-bis(hydroxymethyl)-6,7-diethoxy-1-[1-(2-methoxyethyl)-2-oxo-4-pyridyl]-naphthalene and 2,3-bis(hydroxymethyl)-6,7-diethoxy-1-[2-(4-(3-pyridyl)-1(2H)-phthalazinone-2-yl)-4-pyridyl]-naphthalene, etc. In particular, medicinal compns. containing the PDE4 inhibitor and a biocompatible and biodegradable polymer which exert an excellent effect of repairing cartilage when processed into dosage forms adequate for topical administration to sites suffering from chondropathy, for example, microspherical preps.

IT 209261-43-8

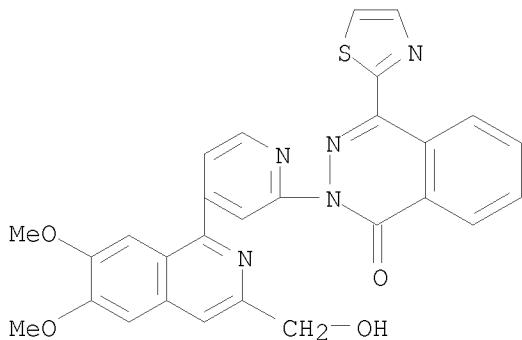
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(therapeutic compns. for repairing chondropathy containing phosphodiesterase 4 inhibitors)

RN 209261-43-8 HCAPLUS

CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-isoquinolinyl]-2-pyridinyl]-4-(2-thiazolyl)- (CA INDEX NAME)

STN



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 20 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:902258 HCPLUS

DOCUMENT NUMBER: 137:379992

TITLE: Method of inhibiting neoplastic cells with isoquinolinonecarboxylates

INVENTOR(S): Pamukcu, Rifat; Piazza, Gary A.

PATENT ASSIGNEE(S): Cell Pathways, Inc., USA

SOURCE: U.S., 119 pp.

CODEN: USXXAM

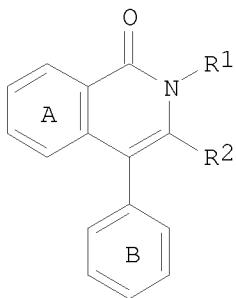
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6486155	B1	20021126	US 1998-198413	19981124 <--
PRIORITY APPLN. INFO.:			US 1998-198413	19981124
OTHER SOURCE(S):	MARPAT	137:379992		
GI				

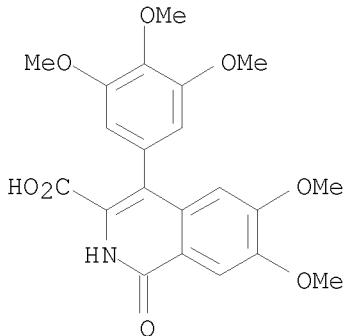


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AB A method is claimed for inhibiting neoplasia (no data), particularly cancerous and precancerous lesions, by exposing the affected cells to 1-isoquinoline-3-carboxylates. Such compds. are effective in modulating

apoptosis and eliminating and inhibiting the growth of neoplasias such as precancerous lesions, but are not characterized by the severe side reactions of conventional non-steroidal antiinflammatory drugs or other chemotherapeutics. Although the methods of preparation are not claimed, example preps. of 429 isoquinolines and 107 intermediates are included; these examples are referenced to PCT application WO 98/38168. Although the claims indicate I (ring A and ring B are the same or different and each a (un)substituted benzene ring, R1 is morpholine, R2 is -COOR₃, and R₃ is alkyl; e.g. 7-benzyloxy-6-methoxy-3-methoxycarbonyl-2-morpholino-4-(3,4,5-trimethoxyphenyl)-1(2H)-isoquinolinone) or pharmaceutically acceptable salt thereof, the examples include a much broader variety of 1-isoquinoline-3-carboxylates.

IT 212489-07-1P, 3-Isoquinolinecarboxylic acid,
1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); USES (Uses)
(preparation of isoquinolinonecarboxylates for inhibiting neoplastic cells)
RN 212489-07-1 HCPLUS
CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-
trimethoxyphenyl)- (CA INDEX NAME)

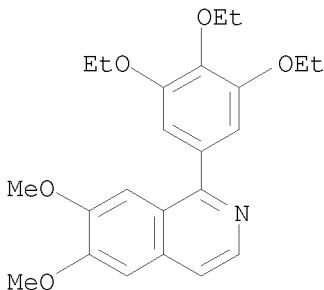


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 171 THERE ARE 171 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L13 ANSWER 21 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:624439 HCPLUS
DOCUMENT NUMBER: 137:129831
TITLE: Method of extracting octaverine from Chinese herbal
medicine Poncirus trifoliata
INVENTOR(S): Hou, Tuanzhang
PATENT ASSIGNEE(S): Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 3 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

STN

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1318538	A	20011024	CN 2001-106994	20010411 <--
PRIORITY APPLN. INFO.:				
AB The method comprises extracting <i>Poncirus trifoliata</i> with water, concentrating, precipitating				
with alc., concentrating, filtering with sand, purifying on cation exchange resin				
column with NH ₄ OH as eluent, concentrating, crystallizing, and recrystg.				
IT 549-68-8, Octaverine	RL: NPO (Natural product occurrence); PEP (Physical, engineering or chemical process); PYP (Physical process); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PROC (Process); USES (Uses)			
RN 549-68-8 HCPLUS	(extracting octaverine from Chinese herbal medicine)			
CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)				



L13 ANSWER 22 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:512253 HCPLUS
DOCUMENT NUMBER: 138:198129
TITLE: Molecular modeling of 3-arylisouinoline antitumor agents active against A-549. A comparative molecular field analysis study
AUTHOR(S): Cho, Won-Jea; Kim, Eui-Ki; Park, Il Yeong; Jeong, Eun Young; Kim, Tae Sung; Le, Thanh Nguyen; Kim, Dae-Duk; Lee, Eung-Seok
CORPORATE SOURCE: Chonnam National University, College of Pharmacy, Kwangju, Buk-gu, 500-757, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(9), 2953-2961
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:198129
AB A series of 58 3-arylisouinoline antitumor agents were investigated for defining the pharmacophore model using comparative mol. field anal. (CoMFA) program. The studied compds. related to bioisostere of benzophenanthridine alkaloid were synthesized and evaluated for antitumor cytotoxicity against human lung tumor cell (A 549). In order to perform the systematic mol. modeling study of these compds., the conformational search was carried out based on the single x-ray crystallog. structure of

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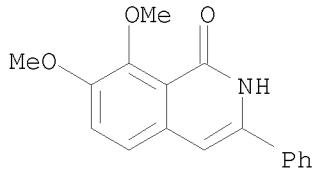
7,8-dimethoxy-3-phenylisoquinolin-(2H)-one. Interestingly, two types of structures having different dihedral angles between the isoquinoline ring and 3-aryl ring were found in the crystals. Therefore, CoMFA was performed two different, overlapping ways. The alignments of the structures were based on the common isoquinoline ring and 3-aryl ring. The 3-D-quant. structure-activity relationship study resulted in significant cross-validated, conventional r² values equal to 0.715 and 0.927, resp.

IT 500582-43-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (mol. modeling of 3-arylisouinoline antitumor agents active against A-549 using a comparative mol. field anal. study)

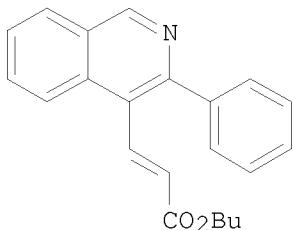
RN 500582-43-4 HCAPLUS

CN 1(2H)-Isoquinolinone, 7,8-dimethoxy-3-phenyl- (CA INDEX NAME)

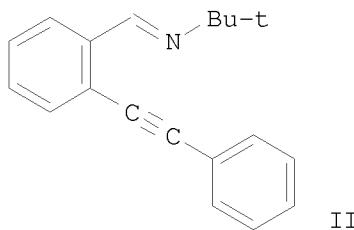


OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 23 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:303956 HCAPLUS
DOCUMENT NUMBER: 137:47095
TITLE: Synthesis of isoquinolines by palladium-catalyzed cyclization, followed by a Heck reaction
AUTHOR(S): Huang, Qinhua; Larock, Richard C.
CORPORATE SOURCE: Department of Chemistry, Iowa State University, Ames, IA, 50011, USA
SOURCE: Tetrahedron Letters (2002), 43(19), 3557-3560
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:47095
GI



I



II

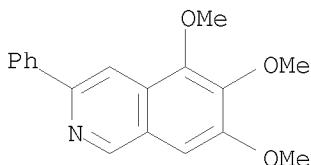
STN

AB A variety of 4-(1-alkenyl)-3-arylisouquinolines, e.g., I, have been prepared by the Pd(II)-catalyzed cyclization of 2-(1-alkynyl)benzaldimines, e.g., II, followed by alkenylation (Heck reaction) in good to excellent yields. The introduction of an ortho-methoxy group on the benzaldimine promotes the Pd-catalyzed cyclization and stabilizes the resulting Pd(II) intermediate improving the yields of the desired isoquinoline products.

IT 438565-15-2P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of isoquinolines via palladium-catalyzed cyclization of alkynylbenzaldimines and subsequent Heck olefination)

RN 438565-15-2 HCPLUS

CN Isoquinoline, 5,6,7-trimethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)

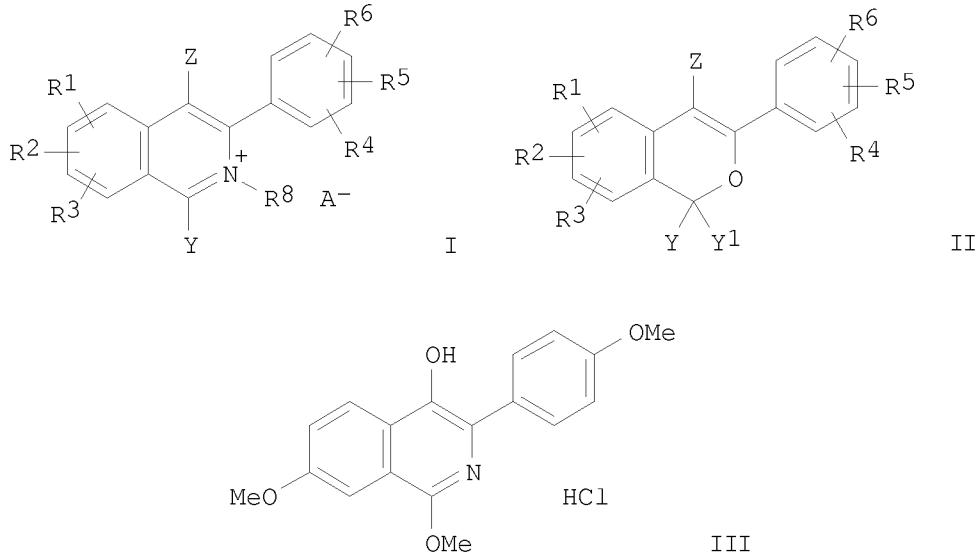
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 24 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:293613 HCPLUS
DOCUMENT NUMBER: 136:309858
TITLE: Preparation of isoquinolines, isochromanones and isothiochromanones as inhibitors of tumor necrosis factor-alpha (TNF-alpha) and/or interleukin-6 (IL-6) and/or cyclooxygenase-2 (COX-2) and/or interleukin-10 (IL-10).
INVENTOR(S): Dey, Debendranath; Neogi, Partha; Sen, Ananda; Sharma, Somesh D.; Nag, Bishwajit
PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002030888	A2	20020418	WO 2001-US31731	20011010 <--
WO 2002030888	A3	20020620		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
CA 2424292 A1 20020418 CA 2001-2424292 20011010 <--
AU 2002011621 A 20020422 AU 2002-11621 20011010 <--
US 20020077333 A1 20020620 US 2001-973190 20011010 <--
US 6723736 B2 20040420
EP 1324994 A2 20030709 EP 2001-979686 20011010 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2004511465 T 20040415 JP 2002-534276 20011010
PRIORITY APPLN. INFO.: US 2000-238475P P 20001010
WO 2001-US31731 W 20011010

OTHER SOURCE(S): MARPAT 136:309858
GI



AB Title compds., e.g. [I, II; R1-R6 = H, (substituted) alkyl, alkenyl, aryl, alkylaryl, alkenylaryl, aryl, CO₂R, etc.; R = H, (substituted) alkyl, alkenyl, aryl, Na, K, Ca, Mg, etc.; R8 = H, OH, (substituted) alkyl, alkenyl, aryl, alkylaryl, alkenylaryl, CO₂R, etc.; Y, Y1 = H, (substituted) alkyl, alkenyl, aryl, alkylaryl, alkenylaryl, CO₂R, etc.; Z = OH, (substituted) alkoxy, amino; A⁻ = pharmaceutically acceptable counterion; with provisos], were prepared Thus, a mixture of 2,3-dimethoxybenzylamine, 4-methoxybenzaldehyde, and NaCN was stirred overnight in Me₂CHOH to give 52% isoquinolinone, which was stirred 48 h in aqueous EtOH open to the atmospheric to give 62.8% title compound (III). III at 1-100 μM inhibited LPS-induced IL-6 production in RAW cells by up to 60%.
IT 343779-66-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

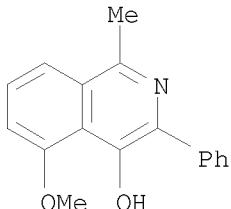
STN

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of isoquinolines, isochromanones and isothiochromanones as
inhibitors of TNF- α and/or IL-6 and/or COX-2 and/or IL-10)

RN 343779-66-8 HCPLUS

CN 4-Isoquinolinol, 5-methoxy-1-methyl-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 25 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:795461 HCPLUS

DOCUMENT NUMBER: 136:69724

TITLE: Synthesis of Isoquinolines and Pyridines by the
Palladium-Catalyzed Iminoannulation of Internal
Alkynes

AUTHOR(S): Roesch, Kevin R.; Zhang, Haiming; Larock, Richard C.

CORPORATE SOURCE: Department of Chemistry, Iowa State University, Ames,
IA, 50011, USA

SOURCE: Journal of Organic Chemistry (2001), 66(24),
8042-8051

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:69724

AB A wide variety of substituted isoquinoline, tetrahydroisoquinoline,
5,6-dihydrobenz[f]isoquinoline, pyrindine, and pyridine heterocycles have
been prepared in good to excellent yields via annulation of internal
acetylenes with the tert-butylimines of o-iodobenzaldehydes and
3-halo-2-alkenals in the presence of a palladium catalyst. The best
results are obtained by employing 5 mol % of Pd(OAc)₂, an excess of the
alkyne, 1 equiv of Na₂CO₃ as a base, and 10 mol % of PPh₃ in DMF as the
solvent. This annulation methodol. is particularly effective for aryl- or
alkenyl-substituted alkynes. When electron-rich imines are employed, this
chemical can be extended to alkyl-substituted alkynes.

Trimethylsilyl-substituted alkynes also undergo this annulation process to
afford monosubstituted heterocyclic products absent the silyl group.

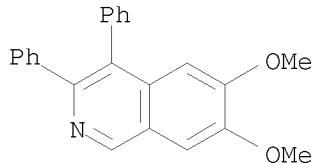
IT 385416-24-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isoquinolines and pyridines by palladium-catalyzed
iminoannulation of internal alkynes)

RN 385416-24-0 HCPLUS

STN

CN Isoquinoline, 6,7-dimethoxy-3,4-diphenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 74 THERE ARE 74 CAPLUS RECORDS THAT CITE THIS RECORD (74 CITINGS)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

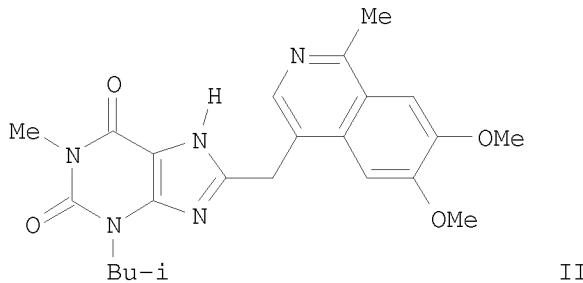
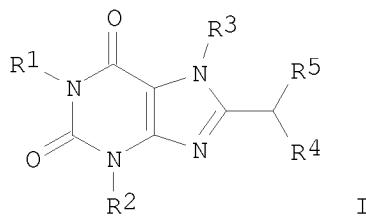
L13 ANSWER 26 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:762998 HCAPLUS
DOCUMENT NUMBER: 135:303908
TITLE: 8-(Quinolinylmethyl)xanthine and 8-(isoquinolinylmethyl)xanthine derivatives as PDE 5 inhibitors, useful for treatment of erectile dysfunction
INVENTOR(S): Bhalay, Gurdip; Collingwood, Stephen Paul; Fairhurst, Robin Alec; Gomez, Sylvie Felicite; Naef, Reto; Sandham, David Andrew
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.
SOURCE: PCT Int. Appl., 70 pp.
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077110	A1	20011018	WO 2001-EP3909	20010405 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2403514	A1	20011018	CA 2001-2403514	20010405 <--
AU 2001073921	A	20011023	AU 2001-73921	20010405 <--
EP 1268480	A1	20030102	EP 2001-940294	20010405 <--
EP 1268480	B1	20031105		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001009855	A	20030603	BR 2001-9855	20010405 <--
HU 2003000565	A2	20030728	HU 2003-565	20010405 <--
HU 2003000565	A3	20041028		

STN

JP 2003530398	T	20031014	JP 2001-575583	20010405
JP 3869725	B2	20070117		
AT 253576	T	20031115	AT 2001-940294	20010405
NZ 521361	A	20040528	NZ 2001-521361	20010405
ES 2210169	T3	20040701	ES 2001-940294	20010405
CN 1176922	C	20041124	CN 2001-807489	20010405
AU 2001273921	B2	20050505	AU 2001-273921	20010405
RU 2269529	C2	20060210	RU 2002-129557	20010405
NO 2002004741	A	20021002	NO 2002-4741	20021002 <--
US 20030171384	A1	20030911	US 2002-240481	20021002 <--
ZA 2002007956	A	20030716	ZA 2002-7956	20021003 <--
IN 2002CN01618	A	20050128	IN 2002-CN1618	20021004
MX 2002009903	A	20030327	MX 2002-9903	20021007 <--
US 20040038996	A1	20040226	US 2003-644328	20030820
US 6919337	B2	20050719		
US 20050054660	A1	20050310	US 2004-937639	20040909
US 7019136	B2	20060328		
US 20060173181	A1	20060803	US 2005-274030	20051115
US 20060106214	A1	20060518	US 2006-329889	20060111
US 7361661	B2	20080422		
PRIORITY APPLN. INFO.:			GB 2000-8694	A 20000407
			WO 2001-EP3909	W 20010405
			US 2002-240481	B1 20021002
			US 2003-644328	A3 20030820
			US 2004-937639	A1 20040909

OTHER SOURCE(S): MARPAT 135:303908
GI



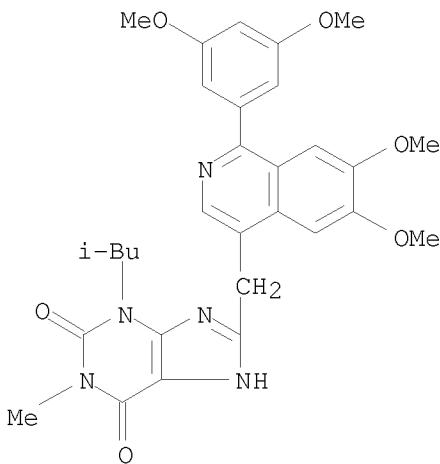
AB Compds. of formula I, in free or salt form, are disclosed [where R1 = H or alkyl (un)substituted by OH, alkoxy, or alkylthio; R2 = H, alkyl, hydroxyalkyl, alkylcarbonyloxyalkyl, alkoxyalkyl, alkylthioalkyl, alkenyl,

cycloalkylalkyl, heterocyclalkyl, aralkyl [aryl ring optionally fused to 5-membered heterocyclic group or substituted by alkoxy, (di)(alkyl)amino, acylamino, halo, OH, aminosulfonyl, alkylaminosulfonyl, dialkylaminosulfonyl, alkylsulfonylamino or dialkylaminosulfonylamino]; R3 = H or alkyl optionally substituted by OH, alkoxy, or alkylthio; R4 = H or alkyl; R5 = (un)substituted quinolinyl, isoquinolinyl, or oxodihydroisoquinolinyl, optionally fused to 5-membered heterocyclic group [substituents = halo, cyano, OH, alkyl, hydroxylalkyl, alkoxyalkyl, alkylthioalkyl, alkoxy, alkylthio, alkenyl, alkoxy carbonyl, alkynyl, carboxyl, acyl, N(R6)R7, (un)substituted aryl (substituents = halo or alkoxy), or 5- or 6-membered heteroaryl attached through ring C]; R6, R7 = H or alkyl (optionally substituted by OH or alkoxy); or 1 of R6 and R7 = H, the other = acyl; or NR6R7 = 5- or 6-membered heterocyclyl]. I are inhibitors of cGMP phosphodiesterases (PDEs), and in particular are selective inhibitors of PDE5. They exhibit good selectivity for PDE5 over PDE1 and PDE6, indicating a low side-effect profile. I are of particular interest for use in the treatment of sexual dysfunction, especially male erectile dysfunction. Examples include 87 product syntheses and 59 intermediate preps. Ten compds. are particularly preferred, and these are specifically claimed. For instance, cyclocondensation of 5,6-diamino-1-isobutyl-3-methyl-1H-pyrimidine-2,4-dione with (6,7-dimethoxy-1-methylisoquinolin-4-yl)acetic acid (preps. given), using EDC in aqueous MeOH, gave the preferred title compound II. In an in vitro assay

for PDE5 inhibition, I gave IC₅₀ values of 0.0005 μM to 10 μM, e.g., 0.007 μM for II.

IT 366444-39-5P, 8-[6,7-Dimethoxy-1-(3,5-dimethoxyphenyl)isoquinolin-4-ylmethyl]-3-isobutyl-1-methyl-3,7-dihydropurine-2,6-dione
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of quinoline-xanthine and isoquinoline-xanthine derivs. as PDE 5 inhibitors)

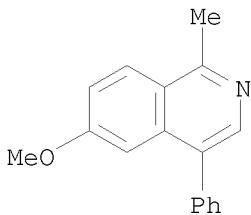
RN 366444-39-5 HCPLUS
 CN 1H-Purine-2,6-dione, 8-[(1-(3,5-dimethoxyphenyl)-6,7-dimethoxy-4-isoquinolinyl)methyl]-3,9-dihydro-1-methyl-3-(2-methylpropyl)-(CA INDEX NAME)



STN

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 27 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:658540 HCAPLUS
DOCUMENT NUMBER: 135:371618
TITLE: Isoquinoline syntheses via Δ 2-oxazolines. Part VIII. Cyclization of 2-acetamido-1,2-diphenylethan-1-ol derivatives into isoquinoline systems
AUTHOR(S): Kopczynski, T.; Voelkel, A.
CORPORATE SOURCE: Institute of Chemical Technology and Engineering, Poznan Technical University, Poznan, 60-965, Pol.
SOURCE: Polish Journal of Chemistry (2001), 75(9), 1317-1325
PUBLISHER: Polish Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:371618
AB The results of the conversion of 2-acetamido-1,2-diphenylethan-1-ol derivs. into 1-methyl-4-phenylisoquinoline derivs. were described. The mechanism proposed for these reaction assumes the existence of protonated Δ 2-oxazolines, carbonium ions, and unsatd. amides as intermediates. For example, the cyclization of erythro-N-(2-hydroxy-1,2-diphenylethyl)acetamide or threo-N-(2-hydroxy-1,2-diphenylethyl)acetamide gave 1-methyl-4-phenylisoquinoline in 66% yield.
IT 374594-09-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isoquinolines via cyclocondensation of N-(hydroxydiphenylethyl)acetamide derivs.)
RN 374594-09-9 HCAPLUS
CN Isoquinoline, 6-methoxy-1-methyl-4-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 28 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:466987 HCAPLUS
DOCUMENT NUMBER: 135:313435
TITLE: Disease activated drugs: a new concept for the treatment of asthma
AUTHOR(S): Charpiot, B.; Bitsch, F.; Buchheit, K.-H.; Channez,

STN

CORPORATE SOURCE: P.; Mazzoni, L.; Mueller, T.; Vachier, I.; Naef, R.
Research, Novartis Pharma AG, Basel, CH-4002, Switz.
SOURCE: Bioorganic & Medicinal Chemistry (2001),
9(7), 1793-1805

PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:313435

AB Disease activated drugs (DAD) are pro-drugs of one active principle or combinations of two drugs, which have a proven efficacy for the treatment of the target disease. In opposition to pro-drugs, DAD are activated in inflamed but not normal tissues. Due to the disease specific activation, the amount of locally released drug(s) should be related directly to the severity of the inflammation. To test this concept in asthma a PDE4 inhibitor, an isoquinoline derivative, was chemical derivatized into pro-drugs

or

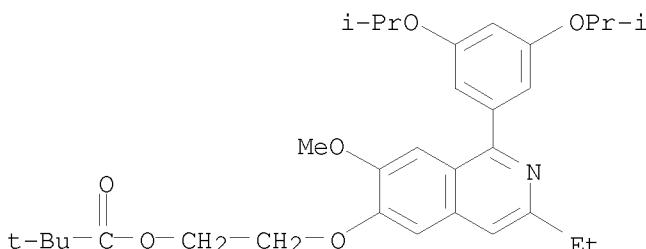
combined with corticosteroids. These new compds. were more readily cleaved into active PDE4 inhibitor, in bronchoalveolar lavage fluid (BALF) from Brown-Norway rats with lung inflammation than in BALF from rats without airway inflammation. The DAD concept (local selective release and improved therapeutic window) was validated *in vivo* using the inhibition of methacholine induced bronchoconstriction in guinea pigs with or without ozone induced lung inflammation. An example of DAD hydrolysis (isoquinoline-dexamethasone) was also examined in BALF from asthmatics and healthy volunteers. PDE4 inhibitors derivatized or combined with steroids were synthesized as DAD models and their cleavage into active PDE4 inhibitors under inflammatory conditions were examined *in vitro*. The DAD concept was also validated in animals, local release and improved therapeutic window were observed

IT 368445-15-2P

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of disease activated drugs that inhibit phosphodiesterase type 4 as a new concept for the treatment of asthma)

RN 368445-15-2 HCPLUS

CN Propanoic acid, 2,2-dimethyl-, 2-[[1-[3,5-bis(1-methylethoxy)phenyl]-3-ethyl-7-methoxy-6-isoquinolinyl]oxy]ethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS

STN

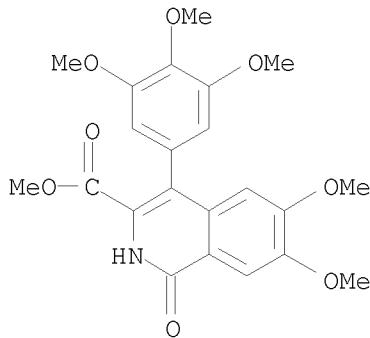
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 29 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:355514 HCPLUS
DOCUMENT NUMBER: 135:76771
TITLE: Novel, potent, and selective phosphodiesterase 5
inhibitors: synthesis and biological activities of a
series of 4-aryl-1-isoquinolinone derivatives
AUTHOR(S): Ukita, Tatsuzo; Nakamura, Yoshinori; Kubo, Akira;
Yamamoto, Yasuo; Moritani, Yasunori; Saruta, Kunio;
Higashijima, Takanori; Kotera, Jun; Takagi, Michino;
Kikkawa, Kohei; Omori, Kenji
CORPORATE SOURCE: Discovery Research Laboratory, Tanabe Seiyaku Co.
Ltd., Yodogawa Osaka, 532-8505, Japan
SOURCE: Journal of Medicinal Chemistry (2001),
44(13), 2204-2218
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:76771
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

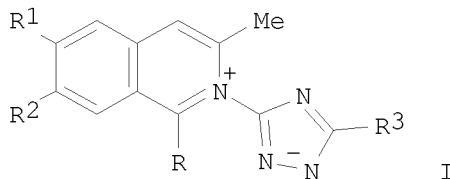
AB A novel class of potent and selective phosphodiesterase 5 (PDE5) inhibitors, the hydrochlorides of 4-aryl-1-isoquinolinone derivs. such as I (R = H, cyclopentyl, morpholino, etc.) designed by the comparison of the structure of cGMP and a previously reported 1-arylnaphthalene lignan, was disclosed. 4-Aryl-1-isoquinolinone derivs. such as the hydrochlorides of I (R = H, cyclopentyl, morpholino, etc.) were prepared and studied as potent and selective inhibitors of phosphodiesterase 5 (PDE5). I were designed by anal. of the structures of cGMP and a previously reported 1-arylnaphthalene lignan. Among these compds., the dihydrochloride of Me 2-(4-aminophenyl)-1,2-dihydro-1-oxo-7-(2-pyridinylmethoxy)-4-(3,4,5-trim ethoxyphenyl)-3-isoquinoline carboxylate (II) exhibited potent PDE5 inhibitory activity ($IC_{50} = 1.0$ nM) with high isoenzyme selectivities (IC_{50} ratio: PDE1/PDE5 = 1300, PDE2/PDE5 > 10 000, PDE3/PDE5 > 10 000, PDE4/PDE5 = 4700, PDE6/PDE5 = 28). Compound II also showed the most potent relaxant effect on isolated rabbit corpus cavernosum ($EC_{30} = 7.9$ nM). Isoquinolinone compound III (T-1032), the sulfate salt of II, was selected for further biol. and pharmacol. evaluation of erectile dysfunction.

IT 212489-49-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of arylisoquinolinone derivs. as selective inhibitors of phosphodiesterase 5 and as potential agents for the treatment of erectile dysfunction)
RN 212489-49-1 HCPLUS
CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 31 THERE ARE 31 CAPLUS RECORDS THAT CITE THIS RECORD (32 CITINGS)
 REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 30 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2001:341939 HCAPLUS
 DOCUMENT NUMBER: 135:122453
 TITLE: On triazoles XLIII[1]. Synthesis of 1,2,4-triazolyl isoquinolinium zwitter ions
 AUTHOR(S): Prauda, Ibolya; Kovacs, Istvan; Trinka, Peter;
 Reiter, Jozsef
 CORPORATE SOURCE: Egis Pharmaceuticals Ltd., Budapest, H-1475, Hung.
 SOURCE: Journal of Heterocyclic Chemistry (2001),
 38(2), 403-414
 CODEN: JHTCAD; ISSN: 0022-152X
 PUBLISHER: HeteroCorporation
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:122453
 GI



AB Isoquinolinium zwitter ions (I) [R1, R2 = OMe, OCH2O; R = Me, (un)substituted phenyl; R3 = H, thioalkyl, alkyl amino, cyclohexylamino, phenylamino, benzylamino, piperidinyl, morpholinyl, substituted piperazinyl] were synthesized by the reaction of ortho-acylphenylacetones or pyrylium salts with different 5-amino-3-substituted-1H-1,2,4-triazoles. Spectroscopic and X-ray diffraction evidence was given for the zwitter ion structure of the products obtained. The position of the neg. charge on the 1,2,4-triazolium ring was proved by comparison of the cmr and uv spectra of the products obtained with the three possible N-benzyl derivs.

STN

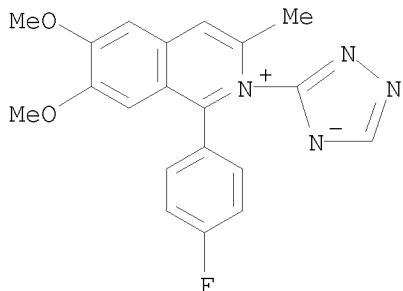
prepared for this purpose.

IT 351207-06-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 1,2,4-triazolyl isoquinolinium zwitter ions)

RN 351207-06-2 HCPLUS

CN Isoquinolinium, 1-(4-fluorophenyl)-6,7-dimethoxy-3-methyl-2-(1H-1,2,4-triazol-5-yl)-, inner salt (CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 31 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:223223 HCPLUS

DOCUMENT NUMBER: 135:46141

TITLE: Synthesis of novel type pyrazolyl- and tetrazolylisoquinolinium zwitterions

AUTHOR(S): Prauda, Ibolya; Reiter, Jozsef

CORPORATE SOURCE: Egis Pharmaceuticals Ltd., Budapest, 1475, Hung.

SOURCE: Journal of Heterocyclic Chemistry (2001), 38(1), 199-204

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:46141

AB N-pyrazol-3-ylisoquinolinium.HCl and N-tetrazol-5-ylisoquinolinium zwitterions were synthesized. Their structures were proved by IR, 1H- and 13C NMR, mass spectra, as well as x-ray diffraction anal. of model compds.

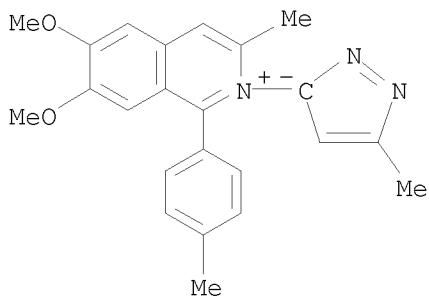
IT 344452-47-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure)

RN 344452-47-7 HCPLUS

CN Isoquinolinium, 6,7-dimethoxy-3-methyl-1-(4-methylphenyl)-2-(5-methyl-3H-pyrazol-3-yl)-, inner salt (CA INDEX NAME)

STN



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 32 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:177271 HCAPLUS

DOCUMENT NUMBER: 135:33424

TITLE: Competitive 3+2 and 2+2 cycloadditions of ester-stabilized azaallyl anions to benzyne. Ring expansion of initial 3+2 products to isoquinolin-3-ones

AUTHOR(S): Hussain, H.; Kianmehr, E.; Durst, T.

CORPORATE SOURCE: Department of Chemistry, University of Ottawa, Ottawa, K1N 6N5, Can.

SOURCE: Tetrahedron Letters (2001), 42(12), 2245-2248

CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:33424

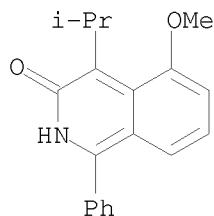
AB Reaction of the azaallyllithiums derived from imines of α -amino esters with benzyne results in the formation of 1,3-dihydroisoindoles and 4-hydroxyisoquinolines via [3+2] and [2+2] cycloaddns., resp. The initially formed 1-carboethoxy-1,3-dihydroisoindoles rearrange under basic reaction conditions to form 3-(2H)-isoquinolinones.

IT 343779-58-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dihydroisoindoles, hydroxyisoquinolines, and isoquinolinones via cycloaddn. of ester-stabilized azaallyl anions to benzyne)

RN 343779-58-8 HCAPLUS

CN 3(2H)-Isoquinolinone, 5-methoxy-4-(1-methylethyl)-1-phenyl- (CA INDEX NAME)



STN

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 33 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:136925 HCAPLUS
DOCUMENT NUMBER: 134:188213
TITLE: Treatment of obstructive airways diseases with
compositions comprising propylsulfonylethylaminoethyl
benzothiazolone and PDE4 inhibitors
INVENTOR(S): Ince, Francis; Dixon, John; Holt, Philip
PATENT ASSIGNEE(S): AstraZeneca UK Limited, UK
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	-----	-----	-----	-----
WO 2001011933	A2	20010222	WO 2000-GB3114	20000814 <--
WO 2001011933	A3	20010614		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000064602	A	20010313	AU 2000-64602	20000814 <--
PRIORITY APPLN. INFO.:			SE 1999-2937	A 19990818
			WO 2000-GB3114	W 20000814

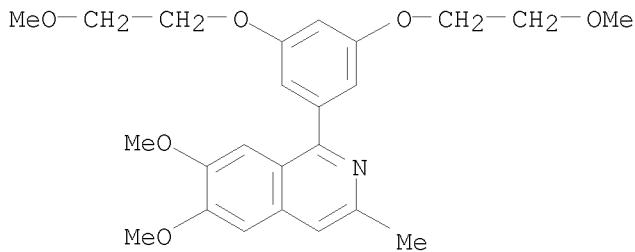
AB The present invention provides a pharmaceutical composition, pharmaceutical product or kit comprising a first active ingredient (A) being 4-hydroxy-7-[2-[2-[3-[2-phenylethoxy]propylsulfonyl]ethylamino]ethyl]-1,3-benzothiazol-2(3H)-one (I) or a pharmaceutically acceptable salt thereof, and a second active ingredient (B) being a PDE4 inhibitor, for use in the treatment of obstructive airways diseases. Antiinflammatory efficacy of a combination of 10 mg/kg oral ariflo and 0.3 g/kg aerosol I was shown in rats.

IT 125175-65-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(treatment of obstructive airways diseases with compns. comprising propylsulfonylethylaminoethyl benzothiazolone and PDE4 inhibitors)

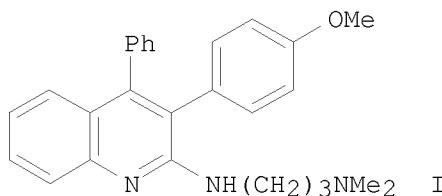
RN 125175-65-7 HCAPLUS

CN Isoquinoline, 1-[3,5-bis(2-methoxyethoxy)phenyl]-6,7-dimethoxy-3-methyl-
(CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 34 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2000:840672 HCPLUS
 DOCUMENT NUMBER: 134:100750
 TITLE: Diphenyl quinolines and isoquinolines: synthesis and primary biological evaluation
 AUTHOR(S): Croisy-Delcey, Martine; Croisy, Alain; Carrez, Daniele; Huel, Christiane; Chiaroni, Angele; Ducrot, Pierre; Bisagni, Emile; Jin, Lu; Leclercq, Guy
 CORPORATE SOURCE: UMR 176 CNRS Institut Curie-Recherche, Laboratoire Raymond Latarjet, UMR 176 CNRS Institut Curie-Recherche, Laboratoire Raymond Latarjet, Centre Universitaire, Orsay, 91405, Fr.
 SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(11), 2629-2641
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:100750
 GI



AB The synthesis of a series of 35 substituted 3,4-di-phenylquinolines and -isoquinolines is described. The majority of these mols. differ from all other triphenylethylene based antiestrogens by a different spatial location of the aminoalkyl side chain. The binding affinity of the most representative mols., including analogs without the side chain, for the estrogen receptor α (ER) was determined. The ability of these mols. to induce the progesterone receptor was also studied. Antiproliferative activity was evaluated on MCF-7 human breast cancer cells, while intrinsic cytotoxic/cytostatic properties resulting from interaction with other targets than ER were assayed on L1210 murine leukemia cells. Introduction

STN

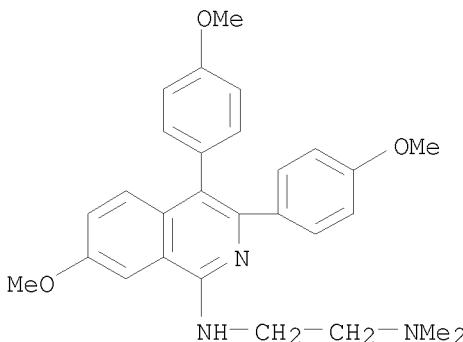
of an aminoalkylamino side chain at carbon 2 confers strong cytotoxic properties to diphenylquinolines as well as pure antiestrogenic activities. However, cytotoxicity is so high with respect to antiestrogenicity that the latter was clearly observable only in one case (I). The structure of I was determined by X-ray crystallog. Mol. modeling of its docking within the hormone-binding domain of the receptor was subsequently undertaken. According to these results, the design of mols. with the side chain bound to the ethylene part of the tri-phenylethylene skeleton might generate compds. of potential pharmacol. interest.

IT 320371-56-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (preparation and cytotoxicity and antiestrogenic activity of diphenylquinolines and -isoquinolines)

RN 320371-56-0 HCPLUS

CN 1,2-Ethanediamine, N2-[7-methoxy-3,4-bis(4-methoxyphenyl)-1-isoquinolinyl]-N1,N1-dimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (22 CITINGS)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 35 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:712977 HCPLUS

DOCUMENT NUMBER: 133:281699

TITLE: Preparation of isoquinoline derivatives as phosphodiesterase V inhibitors

INVENTOR(S): Ukita, Shinzo; Yamada, Koichiro; Ohmori, Kenji; Yoshikawa, Kohei

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 49 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----

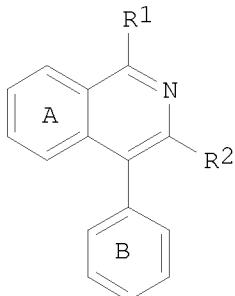
STN

JP 2000281654
PRIORITY APPLN. INFO.:
OTHER SOURCE(S):
GI

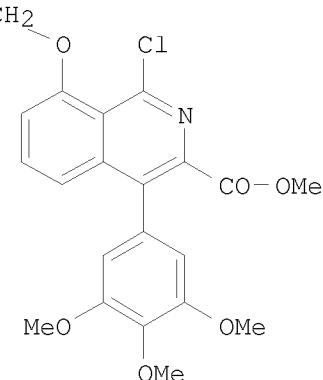
A 20001010

JP 1999-83022

19990326 <--
19990326



T



II

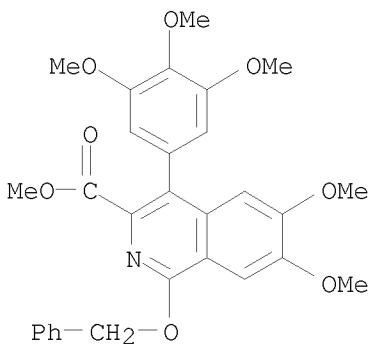
AB The title compds. I [ring A = benzene ring with substituents; ring B = (un)substituted benzene ring; R1 = (un)substituted alkoxy, halo, etc.; R2 = CO₂R₃, etc.; R₃ = H, etc.], useful as phosphodiesterase V inhibitors (no data) for the treatment of circulatory system diseases (no data), are prepared. For example, the title compound II was prepared

IT 299167-15-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinoline derivs. as phosphodiesterase V inhibitors)

RN 299167-15-0 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-(p-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)

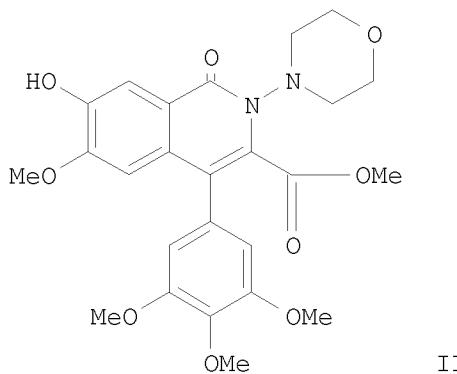
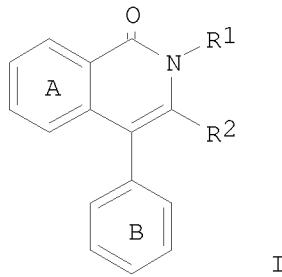


L13 ANSWER 36 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:151451 HCAPLUS
DOCUMENT NUMBER: 132:207769

STN

TITLE: Preparation of isoquinolinones as effective component in medicine
INVENTOR(S): Ukita, Shinzo; Ohmori, Kanji; Ikeo, Tomihiro
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 148 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

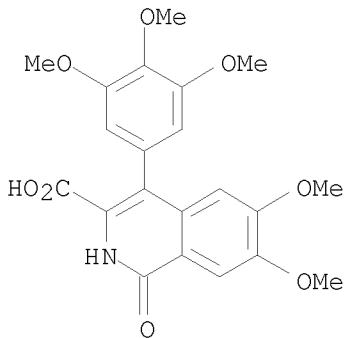
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000072675	A	20000307	JP 1998-240446	19980826 <--
PRIORITY APPLN. INFO.:			JP 1998-240446	19980826
OTHER SOURCE(S): GI	MARPAT	132:207769		



AB Title compds. [I; ring A and ring B equivalent or different, substituted or unsubstituted benzene ring; R1 = H, N(CH₃)₂, 4-H₂NC₆H₄, 4-CH₃OCOC₆H₄, alkyl, cycloalkyl, aryl, complex cyclic; R2 = COOH, COOCH₃, COOCH₂CH₃, COOCH₂C₆H₅, COO(CH₂)₃CH₃] and pharmaceutical acceptable salts are prepared and tested as PDEV inhibitors. The title compound II was prepared
IT 212489-07-1P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

STN

study); PREP (Preparation); USES (Uses)
(preparation of isoquinolinones as effective component in medicine)
RN 212489-07-1 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 37 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:137239 HCAPLUS
DOCUMENT NUMBER: 132:194292
TITLE: Preparation of medicine composition containing pyridylamines
INVENTOR(S): Ukita, Tatsuzo; Sugawara, Masakatsu; Ikezawa, Ichiro;
Yoshikawa, Hideo; Naito, Kazuaki
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 41 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

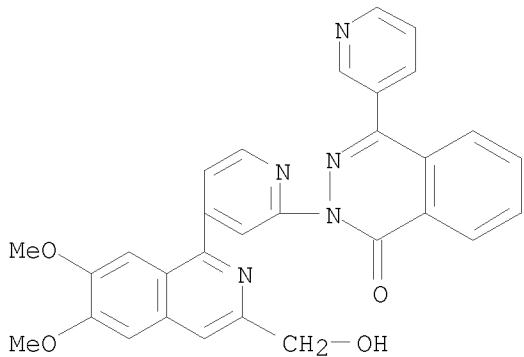
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	-----	-----	-----	-----
JP 2000063275	A	20000229	JP 1999-164565	19990611 <--
PRIORITY APPLN. INFO.:			JP 1998-164045	A 19980612
OTHER SOURCE(S):	MARPAT	132:194292		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; Q = N containing substituted benzoheterocyclic ring; Q1 = N containing substituted benzoheterocyclic ring], stereoisomers, pharmaceutical acceptable salts are prepared as active components in antiasthmatics. The title compound II was prepared
IT 209261-39-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

STN

BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridylamines as antiasthmatics)
RN 209261-39-2 HCPLUS
CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-
isoquinolinyl]-2-pyridinyl]-4-(3-pyridinyl)-, hydrochloride (1:1) (CA
INDEX NAME)

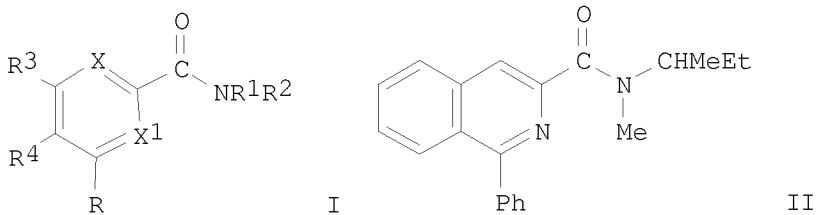


● HCl

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 38 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:732901 HCPLUS
DOCUMENT NUMBER: 131:310567
TITLE: Arene- and heteroarenecarboxamides as benzodiazepine receptors
INVENTOR(S): Dubroeucq, Marie-Christine; Renault, Christian; Le Fur, Gerard
PATENT ASSIGNEE(S): Pharmuka Laboratoires, Fr.
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4499094	A	19850212	US 1983-482082	19830405 <--
FR 2525595	A1	19831028	FR 1982-7217	19820427 <--
FR 2525595	B1	19850322		
PRIORITY APPLN. INFO.: GI			FR 1982-7217	A 19820427



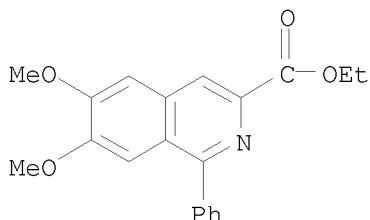
AB Carboxamides I [X, X1 = N, CH; R = Ph, substituted Ph, pyridyl, thienyl; R1, R2 = aliphatic, aromatic; NR1R2 = heterocyclic; R3R4 = (un)substituted CH:CHCH:CH, SCH:CH, CH:CHS] were prepared. Thus 2.4 g II was obtained by amidating 2.96 g of acid with 1.34 g MeNHCHMeEt. II had an affinity for benzodiazepine receptors of 2 nM. The compds. are useful as medicaments for the various applications of benzodiazepines.

IT 89242-43-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of)

RN 89242-43-3 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-phenyl-, ethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 39 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:607187 HCPLUS

DOCUMENT NUMBER: 132:3490

TITLE: Synthesis of isoquino[1,2-a][2]benzazepines and biochemical testing of isomeric homoberbines and related papaverine derivatives on the inhibition of phosphodiesterases

AUTHOR(S): Meise, W.; Onusseit, O.; Clemens, M.

CORPORATE SOURCE: Pharmazeutisches Institut, Univ. Bonn, Bonn, D-53115, Germany

SOURCE: Pharmazie (1999), 54(9), 658-666

CODEN: PHARAT; ISSN: 0031-7144

PUBLISHER: Govi-Verlag Pharmazeutischer Verlag

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 132:3490

STN

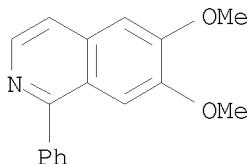
AB A synthesis of hitherto not accessible isoquinolo[1,2-a][2]benzazepines from benzoannelated 7-membered ring lactones or .vepsiln.-hydroxy esters is reported, and their conformation is presented. Testing of these and similar compds. for inhibition of phosphodiesterases showed that the steric arrangement of the benzene rings to each other is important. Due to high deflexion, the homoerbines possess a weak, the norpapaverines a rather good inhibitory activity. For 4,5-dihydro-3 H-2-benzazepines a certain PDE IV-specificity is achieved.

IT 4029-09-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(inhibition by isoquinobenzazepines, homoerbines, and norpapaverines)

RN 4029-09-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 40 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:529842 HCPLUS

DOCUMENT NUMBER: 131:310536

TITLE: Synthesis of 1-(2-Aminophenyl)isoquinolines and the Biological Activity of Their cis-Dichloro Platinum(II) Complexes

AUTHOR(S): von Nussbaum, Franz; Miller, Bernhard; Wild, Stefan; Hilger, Christoph S.; Schumann, Susanne; Zorbas, Haralabos; Beck, Wolfgang; Steglich, Wolfgang

CORPORATE SOURCE: Institut fuer Organische Chemie der Universitaet Muenchen, Munich, D-81377, Germany

SOURCE: Journal of Medicinal Chemistry (1999), 42(18), 3478-3485

PUBLISHER: CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: American Chemical Society

LANGUAGE: Journal

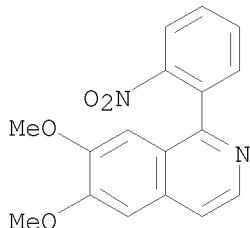
OTHER SOURCE(S): English

CASREACT 131:310536

AB The broad biol. effects of isoquinolines prompted us to use them as chelating, nonleaving ligands in cis-platinum(II) antitumor complexes. The synthesis of several 1-(2-aminophenyl)isoquinoline derivs. with different levels of hydrogenation and varying substitution of the Ph ring is reported. These compds. constitute a new class of ligands for the synthesis of oligocyclic platinum(II) complexes. In vitro cytotoxicity tests indicate that the most basic amine ligands afford the most effective complexes. Two of the new complexes were more potent against L1210 murine leukemia cells than the well-established antitumor compound cisplatinum.

STN

IT 143576-69-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; synthesis of (aminophenyl)isoquinolines and biol.
activity of their cis-dichloro platinum complexes)
RN 143576-69-6 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(2-nitrophenyl)- (CA INDEX NAME)

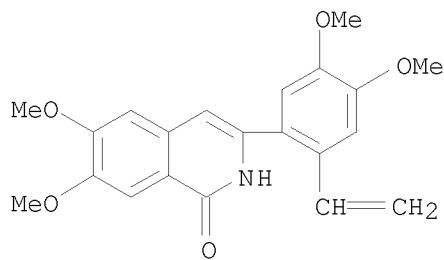


OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 41 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:269393 HCPLUS
DOCUMENT NUMBER: 130:352179
TITLE: Applications of carbon-nitrogen bond cleavage reaction: a synthesis/derivatization of 11H-indeno[1,2-c]isoquinolines
AUTHOR(S): Lal, Banshi; Gidwani, Ramesh M.
CORPORATE SOURCE: Research Center, Hoechst Marion Roussel Limited, Mumbai, 400 080, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1999), 38B(1), 33-39
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:352179
AB Orthophosphoric acid/HCOOH treatment of 3-(4,5-dimethoxy-2-vinylphenyl)-1(2H)-isoquinolinone and 6,7-dimethoxy 3-(4,5-dimethoxy-2-vinylphenyl)-1(2H)-isoquinolinone brings about cyclization to give the indeno[1,2-c]isoquinolines. Reaction with POC13 produces chloro compds. Hydrogenolysis gives dechlorinated products. Reaction of chloro derivs. with different amines gives amino substituted 11H-indeno-[1,2-c]isoquinolines.

IT 60315-12-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and reactions of indenoisoquinolines)
RN 60315-12-0 HCPLUS
CN 1(2H)-Isoquinolinone, 3-(2-ethenyl-4,5-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)

STN



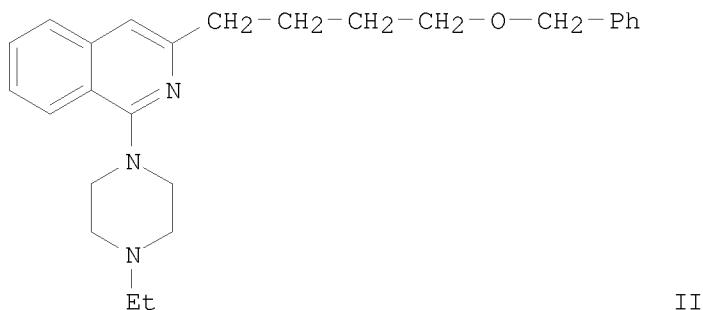
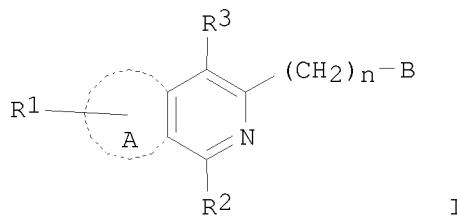
OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 42 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:244638 HCAPLUS
DOCUMENT NUMBER: 130:311813
TITLE: Preparation of piperazinylisoquinolines and analogs as serotonin antagonists
INVENTOR(S): Ueno, Kohshi; Sasaki, Atsushi; Kawano, Koki; Okabe, Tadashi; Kitazawa, Noritaka; Takahashi, Keiko; Yamamoto, Noboru; Suzuki, Yuichi; Matsunaga, Manabu; Kubota, Atsuhiko
PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan
SOURCE: PCT Int. Appl., 740 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9918077	A1	19990415	WO 1998-JP4465	19981002 <--
W: US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2000053647	A	20000222	JP 1998-281752	19981002 <--
JP 3989102	B2	20071010		
EP 1020445	A1	20000719	EP 1998-945593	19981002 <--
EP 1020445	B1	20080813		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 404539	T	20080815	AT 1998-945593	19981002
US 6340759	B1	20020122	US 2000-509778	20000331 <--
US 20020013460	A1	20020131	US 2001-852850	20010511 <--
US 6790844	B2	20040914		
US 20040204421	A1	20041014	US 2004-796673	20040310
US 6875761	B2	20050405		
PRIORITY APPLN. INFO.:				
		JP 1997-284290	A 19971002	
		JP 1998-153416	T0 19980602	
		WO 1998-JP4465	W 19981002	
		US 2000-509778	A3 20000331	
		US 2001-852850	A3 20010511	

STN

OTHER SOURCE(S): MARPAT 130:311813
GI



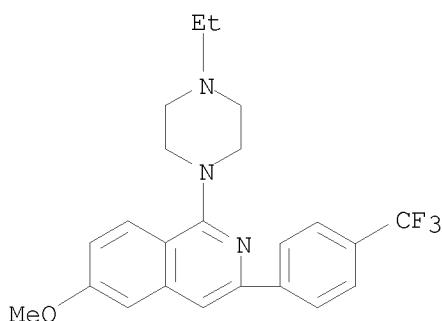
AB The title compds. I [ring A = benzene, pyridine, thiophene or furan ring; B = (un)substituted aryl, etc.; R1 = H, halo, etc.; R2 = 4-morpholinyl, etc.; R3 = H, halo, etc.; n = 0, or 1 - 6] are prepared I are central muscle relaxing drugs for treating, ameliorating or preventing spastic paralysis or ameliorating myotonia. In an in vitro test for 5HT1 receptor antagonism, the title compound II showed the Ki value of 21.2 nM.

IT 223544-97-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperazinylisoquinolines and analogs as serotonin antagonists)

RN 223544-97-6 HCPLUS

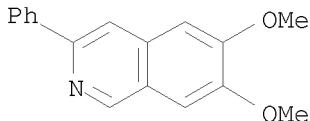
CN Isoquinoline, 1-(4-ethyl-1-piperazinyl)-6-methoxy-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



STN

OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 43 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:39450 HCAPLUS
DOCUMENT NUMBER: 130:196425
TITLE: Electronic spectra of 3-phenyl-6,7-dimethoxyisoquinoline derivatives in polycrystalline state and solution
AUTHOR(S): Kakas, Marija; Janic, Ivan; Kapor, Agnes
CORPORATE SOURCE: Institute of Physics, University of Novi Sad, Novi Sad, Yugoslavia
SOURCE: Physical Chemistry '98, International Conference on Fundamental and Applied Aspects of Physical Chemistry, 4th, Belgrade, Sept. 23-25, 1998 (1998), 137-139. Editor(s): Ribnikar, Slobodan; Anic, Slobodan. Society of Physical Chemists of Serbia: Belgrade, Yugoslavia.
CODEN: 67DYA8
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The absorption (at 293 K), excitation and fluorescence spectra of isoquinoline derivs. (R = H, Me) contribute to the determination of Ph group position and to solving problems that arose in the crystallog. investigation.
IT 24285-10-7
RL: PRP (Properties)
(electronic spectra of 3-phenyl-6,7-dimethoxyisoquinoline derivs. in polycryst. state and solution)
RN 24285-10-7 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-3-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 44 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:608601 HCAPLUS
DOCUMENT NUMBER: 129:216521
ORIGINAL REFERENCE NO.: 129:44019a, 44022a
TITLE: Preparation of 1-isoquinolinone-3-carboxylates as PDE V inhibitors
INVENTOR(S): Ukita, Tatsuzo; Omori, Kenji; Ikeo, Tomihiro
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 299 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

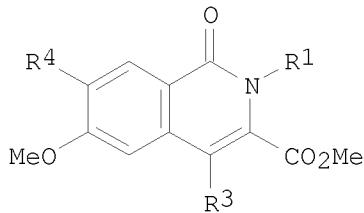
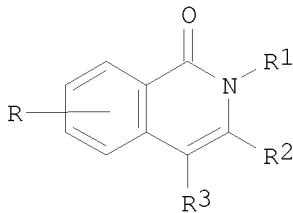
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9838168	A1	19980903	WO 1998-JP715	19980223 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 1998MA00345	A	20050304	IN 1998-MA345	19980220
AU 9862300	A	19980918	AU 1998-62300	19980223 <--
JP 10298164	A	19981110	JP 1998-44139	19980226 <--
PRIORITY APPLN. INFO.:			JP 1997-44408	A 19970227
			WO 1998-JP715	W 19980223

OTHER SOURCE(S): MARPAT 129:216521

GI



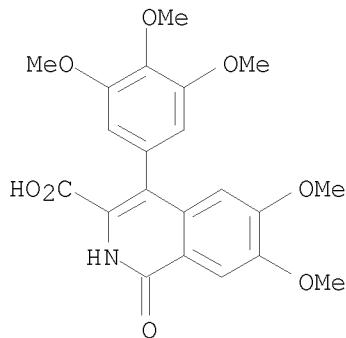
AB Title compds. [I; R = H or substituent(s); R1 = H, NH2, (cyclo)alkyl, heterocyclyl, aryl, etc.; R2 = (esterified) CO2H, CONH2, N-attached heterocyclylcarbonyl, etc.; R3 = (un)substituted Ph] were prepared as PDE V inhibitors (no data). Thus, 5-benzyloxy-4-methoxy-2-(3,4,5-trimethoxybenzoyl)benzoic acid was cyclocondensed with CH2(CO2CMe3)2 and the hydrated product cyclocondensed with 4-(H2N)C6H4NHCO2CMe3 to give, in 4 addnl. steps, title compound II [R1 = C6H4(NH2)-4, R3 = C6H2(OMe)3-3,4,5, R4 = 2-pyridylmethoxy].

IT 212489-07-1P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 1-isoquinolin-3-carboxylates as PDE V inhibitors)

RN 212489-07-1 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)

STN



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 45 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:398243 HCAPLUS
DOCUMENT NUMBER: 129:81741
ORIGINAL REFERENCE NO.: 129:16880h, 16881a
TITLE: Preparation of pyridines as antiasthmatics
INVENTOR(S): Ukita, Tatsuzo; Sugahara, Masakatsu; Ikezawa, Katsuo;
Kikkawa, Hideo; Naito, Kazuaki
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 59 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 848000	A1	19980617	EP 1997-309947	19971210 <--
EP 848000	B1	20020612		
R: AT, BE, CH, IE, SI, LT, DE, DK, ES, FR, LV, FI, RO			GB, GR, IT, LI, LU, NL, SE, MC, PT,	
US 5965730	A	19991012	US 1997-985042	19971204 <--
TW 429257	B	20010411	TW 1997-86118300	19971205 <--
AT 219075	T	20020615	AT 1997-309947	19971210 <--
ES 2178741	T3	20030101	ES 1997-309947	19971210 <--
CA 2224635	A1	19980613	CA 1997-2224635	19971211 <--
CA 2224635	C	20060131		
CN 1184813	A	19980617	CN 1997-125491	19971212 <--
CN 1127498	C	20031112		
JP 10226685	A	19980825	JP 1997-342352	19971212 <--
JP 3951395	B2	20070801		
HK 1012505	A1	20021025	HK 1998-113891	19981217 <--
PRIORITY APPLN. INFO.:			JP 1996-333357	A 19961213
OTHER SOURCE(S):	MARPAT	129:81741		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

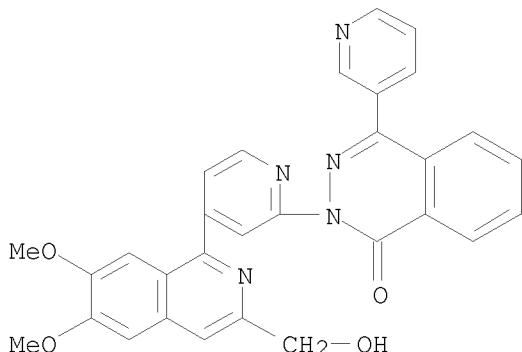
AB The title compds. [I; A = II-VI (wherein R1, R2 = H, (un)protected OH; R31, R41, R42 = (un)protected CH₂OH; R32 = H, lower alkyl, (un)protected CH₂OH; R33 = (un)substituted lower alkyl; the dotted line means the presence or absence of a double bond); R5, R6 = H, (un)protected NH₂, or NR₅R₆ = (un)substituted heterocycle], which show excellent bronchoconstriction inhibitory activity and/or anti-inflammatory activity of airways, and therefore are useful in the prophylaxis or treatment of asthma, were prepared. Thus, reaction of 4-(3-pyridyl)phthalazin-1(2H)-one with 2-bromo-4-[6,7-dimethoxy-2-(4-pyridyl)methyl]phthalazin-1(2H)-one-4-yl]pyridine in the presence of K₂CO₃ and CuI in DMF afforded the title compound VII. Compds. I are effective at 0.003-3 mg/kg/day.

IT 209261-38-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridines as antiasthmatics)

RN 209261-38-1 HCPLUS

CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-1-isoquinolinyl]-2-pyridinyl]-4-(3-pyridinyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(16 CITINGS)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 46 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:211847 HCPLUS

DOCUMENT NUMBER: 128:294669

ORIGINAL REFERENCE NO.: 128:58399a, 58402a

TITLE: Synthesis of 7,12-dihydro-12-phenyl-5H-6,12-methanodibenz[c,f]azocines via N,N-dibenzylphenacylamines

AUTHOR(S): Coskun, Necdet; Buyukuyosal, Levent

CORPORATE SOURCE: Dep. Chem., Uludag Univ., Bursa, 16059, Turk.

SOURCE: Heterocycles (1998), 48(1), 53-59

CODEN: HTCYAM; ISSN: 0385-5414

STN

PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:294669
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB N,N-Dibenzylphenacylamines I (R1 = R2 = MeO, R3 = R4= R5 = R6 = H; R1 = R6 = H, R2 = R3 = R4 = R5 = MeO; R1R2 = OCH2O, R3 = R6 = H, R4 = R5 = MeO; etc.) were prepared in high yields by a one-pot reaction and cyclized at room temperature to give 7,12-dihydro-12-phenyl-5H-6,12-methanodibenz[c,f]azocines II in high yields. 95% H₂SO₄ or 70% HClO₄ was used as cyclization catalysts. The double-cyclization proceeds smoothly in the cases where electron-donating groups are present in both benzene rings. N-2,3-dimethoxybenzyl-N-benzylphenacylamine gave the corresponding N-benzyl-1,2-dihydro-4-phenylisoquinoline on treatment with 95% H₂SO₄ while N-3,4-dimethoxybenzyl-N-benzylphenacylamine at the same reaction conditions and reaction time cyclized to the corresponding dibenzazocine. However, N-3,4-dimethoxybenzyl-N-benzylphenacylamine gave the corresponding dihydroisoquinoline which disproportionates to give N-benzyl-1,2,3,4-tetrahydro-4-phenylisoquinoline and N-benzyl-4-phenylisoquinolinium when treated with 70% perchloric acid at room temperature

IT 206126-10-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phenylmethanodibenzazocines by cyclization of dibenzylphenacylamines)

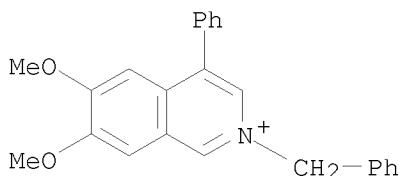
RN 206126-10-5 HCPLUS

CN Isoquinolinium, 6,7-dimethoxy-4-phenyl-2-(phenylmethyl)-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 206126-09-2

CMF C24 H22 N O2

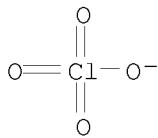


CM 2

CRN 14797-73-0

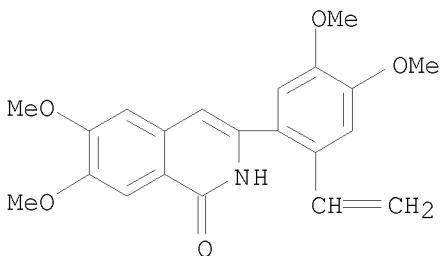
CMF Cl O4

STN



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 47 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:743385 HCAPLUS
DOCUMENT NUMBER: 128:23041
ORIGINAL REFERENCE NO.: 128:4523a, 4526a
TITLE: Applications of a novel carbon-nitrogen bond cleavage reaction. Part IV - a new biomimetic synthesis of benzo[c] phenanthridine alkaloids
Lal, Banshi; Gidwani, Ramesh M.
AUTHOR(S):
CORPORATE SOURCE: Research Center, Hoechst Marion Roussel Limited, Mumbai, 400 080, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1997), 36B(8), 679-681
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A highly practical synthesis of benzo[c]phenanthridine alkaloids nitidine and 2-methoxyfagaronine has been developed from the corresponding protoberberines. The 8-oxoprotoberberines on reaction with NaH and DMF give the C-N bond cleavage intermediates which through a sequence of three reactions are converted into benzo[c]phenanthridine alkaloids.
IT 60315-12-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(biomimetic synthesis of benzo[c]phenanthridine alkaloids)
RN 60315-12-0 HCAPLUS
CN 1(2H)-Isoquinolinone, 3-(2-ethenyl-4,5-dimethoxyphenyl)-6,7-dimethoxy-
(CA INDEX NAME)

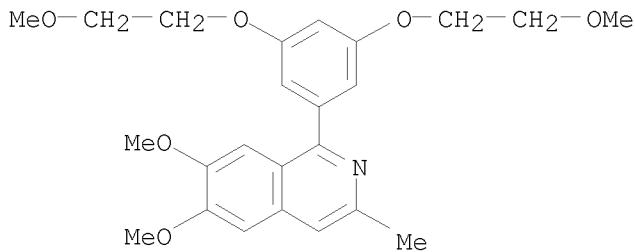


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

STN

L13 ANSWER 48 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:571350 HCPLUS
DOCUMENT NUMBER: 127:274587
ORIGINAL REFERENCE NO.: 127:53541a,53544a
TITLE: Rolipram inhibition of the human cyclic AMP specific phosphodiesterase splice variant HSPDE4D3 expressed in yeast (*Saccharomyces cerevisiae*)
AUTHOR(S): Wilkinson, Ian; Engels, Peter; Houslay, Miles D.
CORPORATE SOURCE: Division Biochemistry Molecular Biology, University Glasgow, Glasgow, G12 8QQ, UK
SOURCE: Pharmacology Reviews and Communications (1997), 9(3), 215-225
CODEN: PHRCF6
PUBLISHER: Harwood
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A PCR procedure was used to generate a cDNA encoding a full length copy of a human cAMP-specific HSPDE4D phosphodiesterase splice variant which was analogous to the rat PDE4D3 form. This cDNA was engineered for expression in a *Saccharomyces cerevisiae* strain where expression of endogenous PDE genes and the major protease cascade were disrupted. Transfection with the plasmid encoding human PDE4D3 rescued this yeast strain from heat shock and led to the expression of cAMP specific PDE activity which was insensitive to Ca²⁺/CaM and low cGMP levels but was profoundly inhibited by the selective PDE4 inhibitor, rolipram. This PDE activity decayed as a single exponential at 45° with a half life (T_{0.5}) of 1.4 min, implying the expression of a single, kinetically homogeneous enzyme. PDE4D3 activity assayed in the presence of 1 μM-cAMP was dose-dependently inhibited by MNS-949, denbufylline, rolipram and theophylline with IC₅₀, values of 0.09, 1.0, 1.9, and 412 μM, resp. Rolipram served as a simple competitive inhibitor of human PDE4D3, yielding a K_i value of 1.3 μM. PDE4D3 was dose-dependently activated by the divalent cation Mg²⁺. In contrast, while Mn²⁺ and Zn²⁺ activated the enzyme at low concns. they inhibited activity at high concns. Ca²⁺ served only to inhibit PDE activity in a dose-dependent manner. Stimulatory concns. of Mg²⁺ affected neither the Km for cAMP nor the form and Ki value seen for rolipram inhibition, suggesting that Mg²⁺ did not affect binding to the active site but achieved activation of PDE4D by increasing the rate of catalysis of the enzyme (V_{max}).
IT 125175-65-7, MNS-949
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (inhibition of the human cAMP specific phosphodiesterase splice variant HSPDE4D3 expressed in *Saccharomyces cerevisiae*)
RN 125175-65-7 HCPLUS
CN Isoquinoline, 1-[3,5-bis(2-methoxyethoxy)phenyl]-6,7-dimethoxy-3-methyl-(CA INDEX NAME)

STN



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

L13 ANSWER 49 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:542447 HCAPLUS
DOCUMENT NUMBER: 127:220851
ORIGINAL REFERENCE NO.: 127:43049a, 43052a
TITLE: Coralyne analogs as topoisomerase inhibitors
INVENTOR(S): Lavoie, Edmond J.
PATENT ASSIGNEE(S): Rutgers, State University of New Jersey, USA; Lavoie, Edmond J.
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9729106	A1	19970814	WO 1997-US1676	19970211 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2241551	A1	19970814	CA 1997-2241551	19970211 <--
AU 9721155	A	19970828	AU 1997-21155	19970211 <--
AU 710070	B2	19990916		
EP 888346	A1	19990107	EP 1997-906466	19970211 <--
EP 888346	B1	20010606		
R: BE, DE, ES, FR, GB, IT, NL, SE, PT				
CN 1211252	A	19990317	CN 1997-192211	19970211 <--
CN 1067070	C	20010613		
HU 9900413	A2	19990528	HU 1999-413	19970211 <--
HU 9900413	A3	20020228		
BR 9707425	A	19990720	BR 1997-7425	19970211 <--
NZ 330705	A	20000327	NZ 1997-330705	19970211 <--
JP 2000504687	T	20000418	JP 1997-528606	19970211 <--
ES 2161442	T3	20011201	ES 1997-906466	19970211 <--
US 6121275	A	20000919	US 1998-117558	19980731 <--
NO 9803669	A	19980923	NO 1998-3669	19980811 <--
PRIORITY APPLN. INFO.:			US 1996-11452P	P 19960212

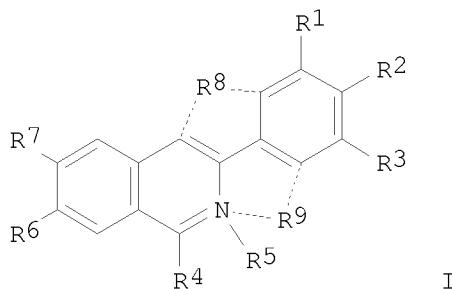
STN

US 1996-32161P P 19961001
WO 1997-US1676 W 19970211

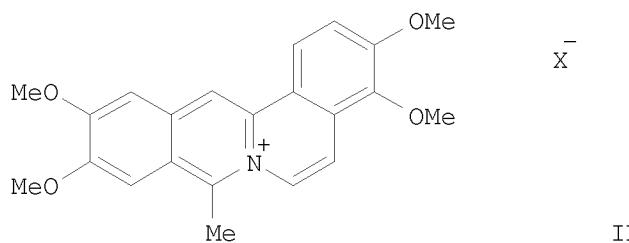
OTHER SOURCE(S):

MARPAT 127:220851

GI



I



II

AB The coralyne derivs. I (R1, R2, R3, R6, R7 = H, OH, alkoxy, R2R3 and R6R7 may form OCH₂O; R4, R5 = H, alkyl; R8, R9 = CH:CH, CH₂CH₂, or ar absent) were prepared as anticancer agents and topoisomerase inhibitors. Thus, the dibenzoquinolizinium derivative II (X = acetosulfate) was pred. in 4 steps. starting from 2,3-dimethoxyphenethylamine and 3,4-dimethoxyacetyl chloride. via cyclization of N-(2,3-dimethoxyphenethyl)-2-(3,4-dimethoxyphenyl)acetamide and 5,6-dimethoxy-1-(3,4-dimethoxybenzyl)isoquinoline hydrochloride. The cytotoxicity IC₅₀ of II (X = acetosulfate) against RPMI cell lines was .4 μ M.

IT 35989-93-6P

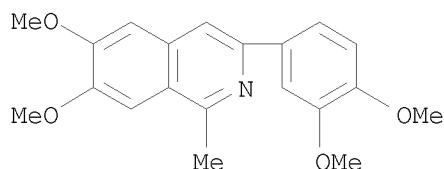
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of Coralyne analogs as topoisomerase inhibitors)

RN 35989-93-6 HCPLUS

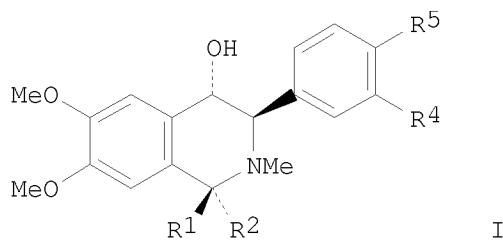
CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)

STN

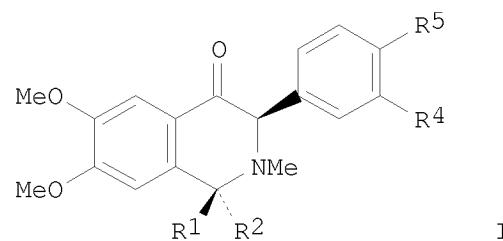


OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 50 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:323380 HCAPLUS
DOCUMENT NUMBER: 127:50525
ORIGINAL REFERENCE NO.: 127:9637a,9640a
TITLE: 3-Aryl-4-isoquinolininone derivatives. An efficient oxidative preparation
AUTHOR(S): Sanmartin, Raul; Olivera, Roberto; Carrillo, Luisa;
Tellitu, Imanol; Badia, Maria Dolores; Dominguez,
Esther
CORPORATE SOURCE: Zientzi Fakultatea, Kimika Organikoa Saila, Euskal
Herriko Unibertsitatea, Bilbao, Spain
SOURCE: Synthetic Communications (1997), 27(10),
1643-1652
CODEN: SYNCV; ISSN: 0039-7911
PUBLISHER: Dekker
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:50525
GI



I



II

AB A comparative study of the oxidation of

STN

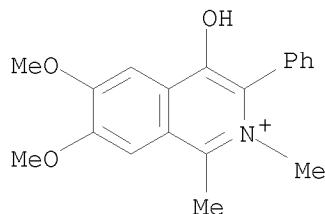
3-aryl-4-hydroxytetrahydroisoquinolines I (R1, R2 = H, Me, R3, R4, R5 = H, OMe) has been carried out. A modification of the Jones conditions turn out to be the best methodol. for the regioselective preparation of target 4-isoquinolinone derivs. II.

IT 190909-96-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation of arylhydroxyisoquinolines to arylisoquinolinones)

RN 190909-96-7 HCPLUS

CN Isoquinolinium, 4-hydroxy-6,7-dimethoxy-1,2-dimethyl-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 51 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1997:322122 HCPLUS

DOCUMENT NUMBER: 127:50524

ORIGINAL REFERENCE NO.: 127:9637a,9640a

TITLE: Preparation of

N-benzylsulfonamido-1,2-dihydroisoquinolines and their reaction with Raney nickel. A mild, new synthesis of isoquinolines

AUTHOR(S): Larghi, Enrique L.; Kaufman, Teodoro S.

CORPORATE SOURCE: Inst. Quimica Organica Sintesis (CONICET-UNR) Fac. Ciencias Bioquimicas Farmaceuticas, Univ. Nacional Rosario, Rosario, 2000, Argent.

SOURCE: Tetrahedron Letters (1997), 38(18), 3159-3162

PUBLISHER: CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Elsevier

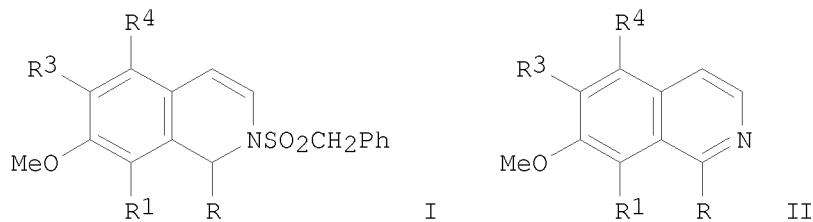
LANGUAGE: Journal

OTHER SOURCE(S): English

CASREACT 127:50524

GI

STN



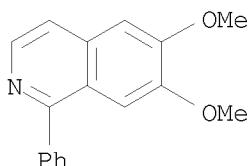
AB N-benzylsulfonamido-1,2-dihydroisoquinolines I (R = H, Me, Et, Ph, 4-MeC₆H₄CH₂, R¹, R³, R⁴ = H, OMe) react with Raney nickel to provide isoquinolines II in excellent yields and under mild, neutral conditions.

IT 4029-09-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and desulfonylation of (benzylsulfonamido)isoquinolines with Raney nickel)

RN 4029-09-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 52 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1997:186975 HCPLUS

DOCUMENT NUMBER: 126:212053

ORIGINAL REFERENCE NO.: 126:41007a, 41010a

TITLE: Preparation of bis[bi(aryl/heteroaryl)] compounds as inhibitors of leukotriene biosynthesis

INVENTOR(S): Friesen, Richard; Dube, Daniel; Ducharme, Yves; Lepine, Carole; Delorme, Daniel; Hamel, Pierre

PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.

SOURCE: Can. Pat. Appl., 80 pp.

CODEN: CPXXEB

DOCUMENT TYPE: Patent

LANGUAGE: English

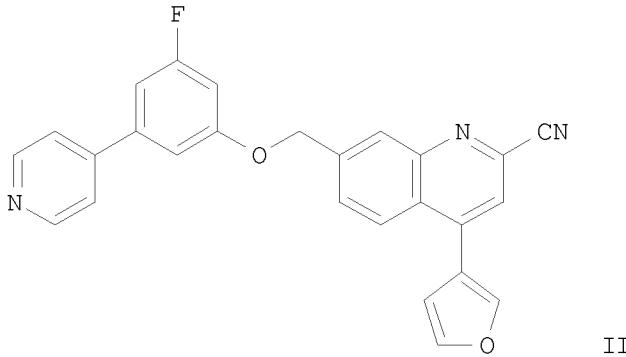
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2169231	A1	19960816	CA 1996-2169231	19960209 <--
US 5576338	A	19961119	US 1995-388787	19950215 <--
PRIORITY APPLN. INFO.:			US 1995-388787	A 19950215

STN

OTHER SOURCE(S): MARPAT 126:212053
GI



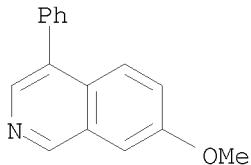
AB The title compds. Ar₁Ar₂-X-Ar₃Ar₄ [I; Ar₁, Ar₄ = (un)substituted 5-membered aromatic ring containing one O or S and 0-3 N, 5-membered aromatic ring containing 1-4 N, 6-membered aromatic ring containing 0-3 N; Ar₂ = (un)substituted arylene = 6-membered aromatic ring containing 0-3 N; Ar₃ = (un)substituted arylene = 10-membered bicyclic aromatic ring containing 0-3 N, 2H-1-benzopyran-2-one, 2H-2-thioxo-1-benzopyran; X = OCH₂, CH₂O, O, S, S(O), S(O)₂], useful as anti-asthmatic, anti-allergic, anti-inflammatory, and cytoprotective agents, and also in treating angina, cerebral spasm, glomerular nephritis, hepatitis, endotoxemia, uveitis, and allograft rejection and in preventing the formation of atherosclerotic plaques, were prepared. Thus, reaction of 3-fluoro-5-(4-pyridyl)phenol with 7-bromomethyl-2-cyano-4-(3-furyl)quinoline in the presence of Cs₂CO₃ in DMF afforded the title compound II. In general, compds. I are effective at 0.1-10 mg/kg/day.

IT 179381-01-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bis[bi(aryl/heteroaryl)] compds. as inhibitors of leukotriene biosynthesis)

RN 179381-01-2 HCPLUS

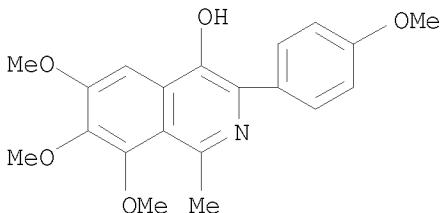
CN Isoquinoline, 7-methoxy-4-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(10 CITINGS)

STN

L13 ANSWER 53 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:662448 HCAPLUS
DOCUMENT NUMBER: 126:31516
ORIGINAL REFERENCE NO.: 126:6417a,6420a
TITLE: A convenient access to protoberberine derivatives
AUTHOR(S): Tellitu, Imanol; Badia, Dolores; Dominguez, Esther;
Carrillo, Luisa
CORPORATE SOURCE: Departamento Quimica Organica, Facultad Ciencias,
Univ. Pais Vasco, Bilbao, Spain
SOURCE: Heterocycles (1996), 43(10), 2099-2112
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A synthesis of protoberberine derivs. starting from (1R*,3S*,4R*)-3-aryl-1-methyl-4-silyloxytetrahydroisoquinolines is presented. The influence of the substitution pattern of the aryl ring at C-3 and the effect of the derivatization of the hydroxyl group at C-4 on the final cyclization reaction is discussed.
IT 184418-07-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of protoberberine derivs. from arylmethylsilyloxytetrahydroisoquinolines)
RN 184418-07-3 HCAPLUS
CN 4-Isoquinolinol, 6,7,8-trimethoxy-3-(4-methoxyphenyl)-1-methyl- (CA INDEX NAME)

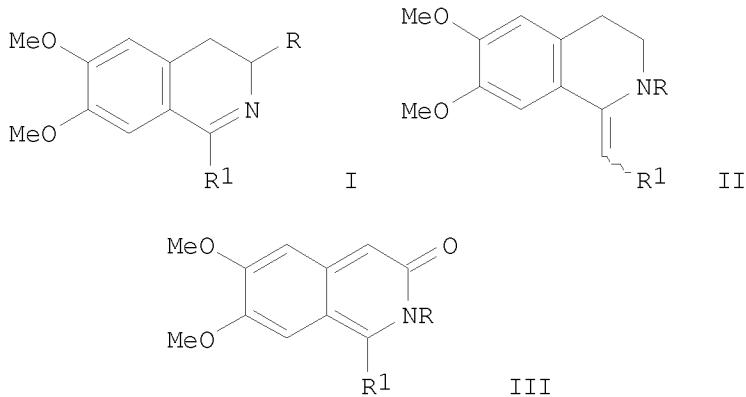


OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

L13 ANSWER 54 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:573452 HCAPLUS
DOCUMENT NUMBER: 125:301283
ORIGINAL REFERENCE NO.: 125:56403a,56406a
TITLE: Synthesis of isoquinolines from 2-phenylethylamines, amides, nitriles and carboxylic acids in polyphosphoric acid
AUTHOR(S): Venkov, Atanas P.; Ivanov, Ilian I.
CORPORATE SOURCE: Dep. Chemistry, Univ. Plovdiv, Plovdiv, 4000, Bulg.
SOURCE: Tetrahedron (1996), 52(37), 12299-12308
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:301283

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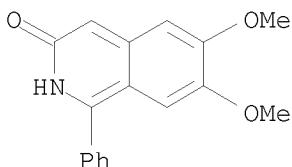
AB A convenient one pot synthesis of C-1 substituted and C-1,3-disubstituted 3,4-dihydroisoquinolines I [R = H, 3,4-(MeO)2C6H3, 4-MeOC6H4, R1 = Me, Ph, Me, PhCH2, etc.], enamines II (R = Me, PhCH2, 4-O2NC6H4CH2, 4-C1C6H4CH2, R1 = Ph), 3-oxo-2,3-dihydroisoquinolines III (R = H, Me, 4-O2NC6H4, R1 = Me, Ph, 4-C1C6H4CH2, 4-O2NC6H4CH2), and enamides II (R = CO2Et, MeCO, MeSO2, 4-O2NC6H4CO, R1 = H, Ph) from 2-phenyl-, 1,2-diphenylethylamines, phenylacetamides, phenylacetonitriles, N-acetylphenylethylamines and carboxylic acids in nonaq. media has been accomplished. The procedures were applied to the synthesis of alkaloids (\pm)-carnegine, N-methylcorydaldine, and xylopinine.

IT 89721-03-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isoquinolines and alkaloids by condensation of phenylethylamines and -amides with carboxylic acids)

RN 89721-03-9 HCPLUS

CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 27 THERE ARE 27 CAPLUS RECORDS THAT CITE THIS RECORD (27 CITINGS)

L13 ANSWER 55 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:476650 HCPLUS

DOCUMENT NUMBER: 125:142577

ORIGINAL REFERENCE NO.: 125:26685a, 26688a

TITLE: Bisarylcarbinol derivatives as inhibitors of leukotriene biosynthesis

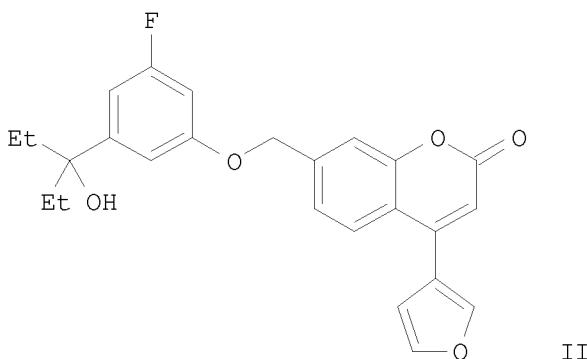
INVENTOR(S): Delorme, Daniel; Ducharme, Yves; Friesen, Richard;

STN

PATENT ASSIGNEE(S): Grimm, Erich L.; Lepine, Carole; Dube, Daniel
Merck Frosst Canada Inc., Can.
SOURCE: PCT Int. Appl., 119 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATIENT INFORMATION:

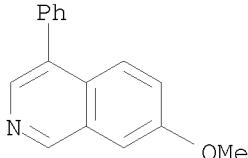
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9613500	A1	19960509	WO 1995-CA608	19951025 <--
W: AL, AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5552437	A	19960903	US 1994-330036	19941027 <--
CA 2203417	A1	19960509	CA 1995-2203417	19951025 <--
CA 2203417	C	20071002		
AU 9536957	A	19960523	AU 1995-36957	19951025 <--
AU 689656	B2	19980402		
EP 788497	A1	19970813	EP 1995-944792	19951025 <--
EP 788497	B1	20010523		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 10507767	T	19980728	JP 1995-514209	19951025 <--
ES 2156961	T3	20010801	ES 1995-944792	19951025 <--
PRIORITY APPLN. INFO.:			US 1994-330036	A1 19941027
			WO 1995-CA608	W 19951025
OTHER SOURCE(S):	CASREACT 125:142577; MARPAT 125:142577			
GI				



AB Compds. having the formula (I): R1R2C(OR3)-Ar1-X-Ar2-Ar3 are inhibitors of leukotriene biosynthesis (no data) [wherein Ar1 = 6-membered aromatic ring containing 0-3 N, and substituted with 1-2 R4 groups; Ar2 = 10-membered bicyclic ring with 1-2 R5 groups (ring system is bicyclic aromatic with 0-4

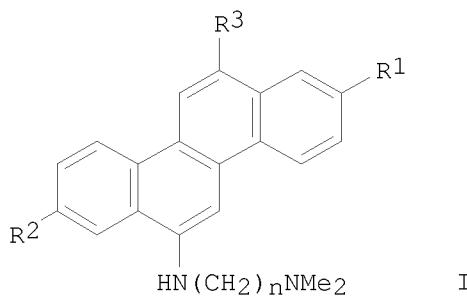
N, or 2H-1-benzopyran-2-one, or 2H-2-thioxo-1-benzopyran); Ar3, Ar4 = 5-membered aromatic with 1 O or S and 0-3 N, or with 1-4 N, or a 6-membered aromatic with 0-3 N, all with 1-2 R6 groups; X = OCH2, CH2O, O, S, S(O), S(O)2; R1 = H, alkyl, perfluoroalkyl, Ar4; R2 = H, alkyl, perfluoroalkyl; R3 = H, alkyl; R4 = H, alkyl, alkoxy, alkylthio, NO2, cyano, CF3, CF3O, halo; R5 = R4, oxo, thioxo; R6 = R4, alkylsulfinyl, alkylsulfonyl, CO2R7; R7 = H, alkyl]. The compds. are useful as antiasthmatic, antiallergic, antiinflammatory, and cytoprotective agents, and are useful for treating angina, cerebral spasm, glomerular nephritis, hepatitis, endotoxemia, uveitis, and allograft rejection, and in preventing the formation of atherosclerotic plaques. Approx. 75 specific examples of I are given. For instance, etherification of 5-fluoro-3-(3-hydroxypent-3-yl)phenol with 7-(bromomethyl)-4-(furan-3-yl)coumarin [preps. given] using Cs2CO3 in DMF at room temperature gave 89% title compound II.

IT 179381-01-2P, 7-Methoxy-4-phenylisoquinoline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of bisarylcarbinol derivs. as leukotriene biosynthesis inhibitors)
 RN 179381-01-2 HCPLUS
 CN Isoquinoline, 7-methoxy-4-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
 REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 56 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1996:474779 HCPLUS
 DOCUMENT NUMBER: 125:221647
 ORIGINAL REFERENCE NO.: 125:41428h, 41429a
 TITLE: A convenient way to dibenzo[c,h]-1,5-naphthyridines (11-aza-benzo[c]phenanthridines)
 AUTHOR(S): Bisagni, Emile; Landras, Corinne; Thirot, Sylvie;
 Huel, Christiane
 CORPORATE SOURCE: Section Recherche, Inst. CURIE, Orsay, 91405, Fr.
 SOURCE: Tetrahedron (1996), 52(31), 10427-10440
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 125:221647
 GI



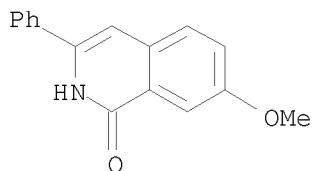
AB Thermal cyclization of variously substituted 2,3-diarylacryloyl azides easily provided a new way to 3-aryl-isoquinolones which were converted to the corresponding 3-aryl-4-nitro-isoquinolones. After reduction into 4-amino-3-aryl-isoquinolones, these were acylated, cyclized, and treated with diamines to give the title compds. I [R1, R2 = H, OMe; R3 = H, Me; n = 2, 3].

IT 62265-91-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dibenzo[c,h]-1,5-naphthyridines)

RN 62265-91-2 HCPLUS

CN 1(2H)-Isoquinolinone, 7-methoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

L13 ANSWER 57 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:432292 HCPLUS

DOCUMENT NUMBER: 125:131653

ORIGINAL REFERENCE NO.: 125:24329a, 24332a

TITLE: Coralyne and related compounds as mammalian

topoisomerase I and topoisomerase II poisons

AUTHOR(S): Makhey, Darshan; Gatto, Barbara; Yu, Chiang; Liu, Angela; Liu, Leroy F.; LaVoie, Edmond J.

CORPORATE SOURCE: Dep. Pharmaceutiacl Chem., Rutgers, State Univ. New Jersey, Piscataway, NJ, 08855, USA

SOURCE: Bioorganic & Medicinal Chemistry (1996), 4(6), 781-791

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB DNA topoisomerases are nuclear enzymes responsible for modifying the topol. state of DNA. The development of agents capable of poisoning

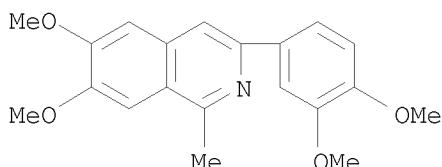
topoisomerase has proved to be an attractive approach in the search for novel cancer chemotherapeutics. Coralyne, an antileukemic alkaloid, has appreciable structural similarity to the potent topoisomerase I and II position, nitidine. Analogs of coralyne were synthesized and evaluated for their activity as topoisomerase I and topoisomerase II poisons. These analogs were also evaluated for cytotoxicity in the human lymphoblast cell line, RPMI 8402, and its camptothecin-resistant variant, CPT-K5. The pharmacol. activity of these analogs exhibited a strong dependence on the substitution pattern and the nature of substituents. Several 1-benzylisoquinolines and 3-phenylisoquinolines were also synthesized. These compds., which incorporate only a portion of the ring structure of coralyne, were evaluated as topoisomerase poisons and for cytotoxicity. These structure-activity studies indicate that the structural rigidity associated with the coralyne ring system may be critical for pharmacol. activity. The presence of a 3,4-methylenedioxy substituent on these coralyne analogs was generally associated with enhanced activity as a topoisomerase poison. 5,6-Dihydro-3,4-methylenedioxy-10,11-dimethoxydibenzo[a,g]quinolizinium chloride was the most potent topoisomerase I poison among the coralyne analogs evaluated, having similar activity to camptothecin. This analog also possessed exceptional potency as a topoisomerase II poison. Despite the pronounced activity of several of these coralyne derivs. as topoisomerase I poisons, none of these compds. had cytotoxic activity similar to camptothecin. Possible differences in cellular absorption between these coralyne analogs, which possess a quaternary ammonium group, and camptothecin may be responsible for the differences observed in their relative cytotoxicity.

IT 35989-93-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation and structure-activity relations of coralyne analogs as topoisomerase I and II poison and cytotoxic agents)

RN 35989-93-6 HCPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 48 THERE ARE 48 CAPLUS RECORDS THAT CITE THIS RECORD (48 CITINGS)

L13 ANSWER 58 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:272796 HCPLUS

DOCUMENT NUMBER: 125:24962

ORIGINAL REFERENCE NO.: 125:4703a,4706a

TITLE: Spectral study of copper(II) flufenamates: crystal and molecular structure of bis(flufenamato)di(N,N-diethylnicotinamide)di(aqua)copper(II)

AUTHOR(S): Melnik, Milan; Potocnak, Ivan; Macaskova, Lubov;
 Miklos, Dusan; Holloway, Clive E.
 CORPORATE SOURCE: Department of Inorganic Chemistry, Slovak Technical
 University, Bratislava, SL 812 37, Slovakia
 SOURCE: Polyhedron (1996), 15(13), 2159-64
 CODEN: PLYHDE; ISSN: 0277-5387
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

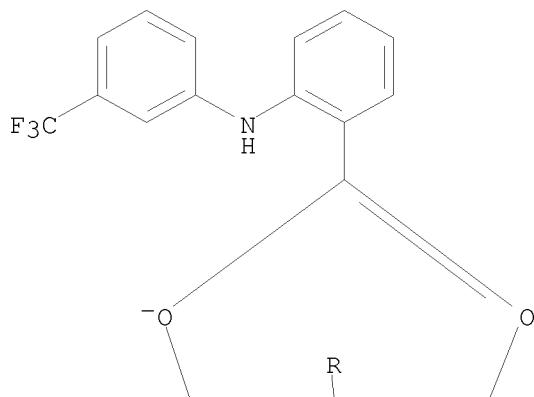
AB New copper(II) flufenamate ($\text{Hflu} = \text{flufenamic acid} = \text{F}_3\text{C}-\text{m-C}_6\text{H}_4\text{NH}-\text{o-C}_6\text{H}_4\text{COOH}$) compds. $\text{Cu}(\text{flu})_2\text{L}$ ($\text{L} = \text{papaverine or caffeine}$) and $\text{Cu}(\text{flu})_2\text{L}_2$ [$\text{L} = \text{nicotine, nicotinamide, N,N-diethylnicotinamide}$ (Et_2nia), pyridine-2,6-dimethanol or $\text{Me-3-pyridylcarbamate}$] were prepared. The spectroscopic properties of $\text{Cu}(\text{flu})_2\text{L}$ indicate copper(II) dimers structurally similar to those in copper(II) acetate monohydrate. All the $\text{Cu}(\text{flu})_2\text{L}_2$ compds. seem to possess octahedral copper(II) stereochem. with differing tetragonal distortions. An x-ray anal. of $\text{Cu}(\text{flu})_2(\text{Et}_2\text{nia})_2(\text{H}_2\text{O})_2$ was carried out, and it featured tetragonal bipyramidal geometry around the copper(II) atom. The tetragonal plane is created by flufenamate anions bonded to the copper(II) atom via the unidentate carboxylate oxygen atoms [$\text{Cu-O}(3) = 196.1(2)$ pm], the pyridine ring nitrogen atoms of the neutral ligand N,N-diethylnicotinamide [$\text{Cu-N}(1) = 200.1(3)$ pm] and axial water mols. [$\text{Cu-O}(2) = 244.9(4)$ pm].

IT 177663-98-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

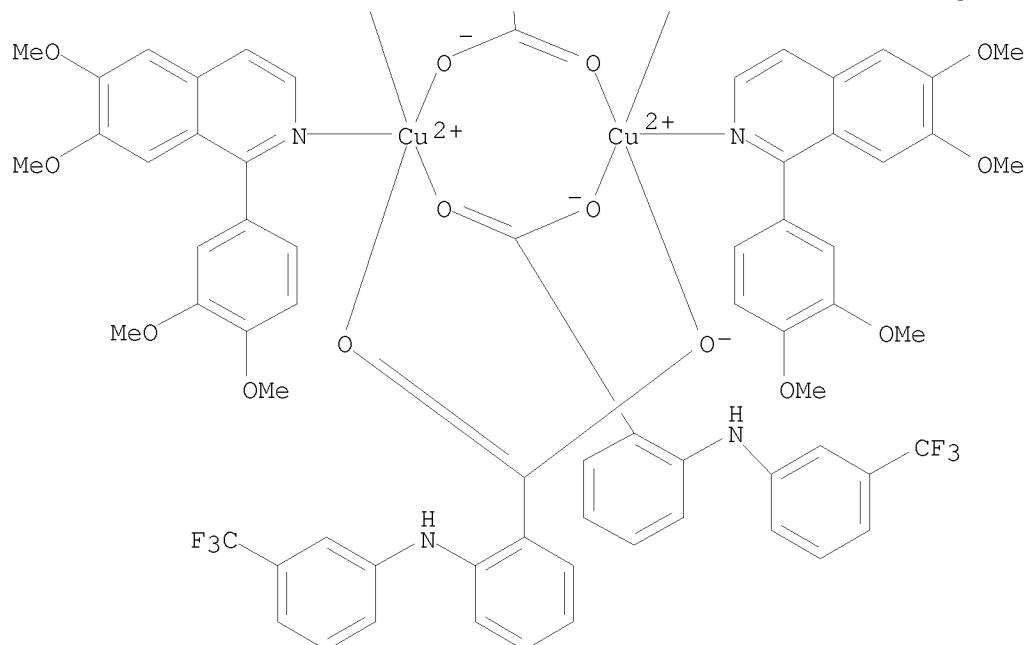
RN 177663-98-8 HCPLUS

CN Copper, bis[1-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline- κN]tetrakis[μ -[2-[3-(trifluoromethyl)phenyl]amino]benzoato- $\kappa\text{O};\kappa\text{O}'$]di-, (Cu-Cu) (9CI) (CA INDEX NAME)

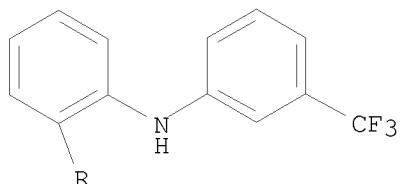
PAGE 1-A



PAGE 2-A



PAGE 3-A



OS.CITING REF COUNT: 41 THERE ARE 41 CAPLUS RECORDS THAT CITE THIS RECORD (41 CITINGS)

L13 ANSWER 59 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1996:206265 HCAPLUS
 DOCUMENT NUMBER: 124:307215
 ORIGINAL REFERENCE NO.: 124:56647a, 56650a
 TITLE: Cyclic AMP promotes the survival of dopaminergic neurons in vitro and protects them from the toxic effects of MPP+
 AUTHOR(S): Hulley, P.; Hartikka, J.; Lubbert, H.
 CORPORATE SOURCE: Preclinical Research, Sandoz Pharma Ltd, Basel, Switz.
 SOURCE: Journal of Neural Transmission, Supplement (1995), 46 (Parkinsons Disease: Experimental

STN

Models and Therapy), 217-28
CODEN: JNTSD4; ISSN: 0303-6995

PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors have studied how stimulation of protein kinase C and cAMP-dependent protein kinases affect the development of mesencephalic dopaminergic neurons in vitro. Insulin-like growth factor-I (IGF-I) and basic fibroblast growth factor (bFGF) did not activate either second messenger system nor affect the survival of dopaminergic neurons but stimulated average dopamine uptake per neuron. Phorbol esters, which stimulate protein kinase C, had no effect on dopamine uptake. Dibutyryl-cAMP caused an increase in dopamine uptake, which was blocked with (Rp)-cAMPS, a specific inhibitor of cAMP-dependent protein kinases. Treating cells with specific phosphodiesterase type IV inhibitors elevated the forskolin-induced increase in dopamine uptake. Furthermore, cAMP, but neither bFGF nor activation dependent astrocyte factor (ADAF), was able to prevent the degeneration of dopaminergic neurons induced by MPP+. These results suggest that increased intracellular cAMP protects dopaminergic neurons in situations of stress and therefore reveal novel possibilities for the treatment of Parkinson's disease.

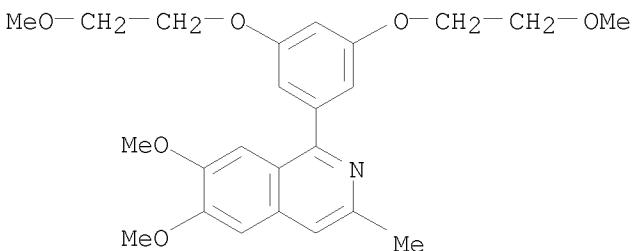
IT 125175-65-7, SDZ-MNS 949

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(increasing cAMP and neurotrophic factors promote survival of mesencephalic dopaminergic neuron cultures in vitro and protects them from toxic effects of MPP+ in relation to protein kinases and Parkinson's disease treatment)

RN 125175-65-7 HCPLUS

CN Isoquinoline, 1-[3,5-bis(2-methoxyethoxy)phenyl]-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

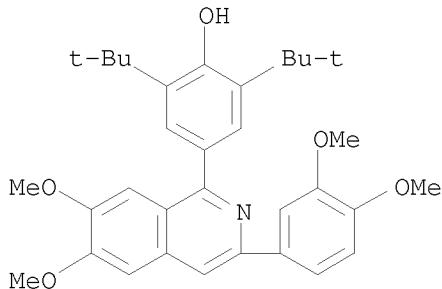
L13 ANSWER 60 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:105836 HCPLUS
DOCUMENT NUMBER: 124:232226
ORIGINAL REFERENCE NO.: 124:43015a, 43018a
TITLE: Sterically hindered 1,4-methylenebenzoquinones in the synthesis of six-membered N-, O-, S- and Se-containing heterocycles
AUTHOR(S): Komissarov, V. N.; Ukhin, L. Yu.; Vetoshkina, L. V.;

STN

CORPORATE SOURCE: Dupin, A. M.; Erin, A. N.
Nauchno-Issled. Inst. Fiz.-Org. Khim., Rostov-on-Don,
Russia
SOURCE: Zhurnal Organicheskoi Khimii (1995), 31(5),
758-64
CODEN: ZORKAE; ISSN: 0514-7492
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 124:232226
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The conversion of quinone methides such as I to heterocycles such as II (X = O, S+O-, Se+O-) and III was described. The isoquinolines possessed high antioxidant activity.
IT 132054-22-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(conversion of quinone methides to heterocycles)
RN 132054-22-9 HCPLUS
CN Phenol, 4-[3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-isoquinolinyl]-2,6-bis(1,1-dimethylethyl) - (CA INDEX NAME)



L13 ANSWER 61 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:948817 HCPLUS
DOCUMENT NUMBER: 124:145854
ORIGINAL REFERENCE NO.: 124:27121a, 27124a
TITLE: Oxidation reactions of 2'-functionalized
3-aryltetrahydro- and 3,4-dihydroisoquinolines
AUTHOR(S): Sotomayor, Nuria; Dominguez, Esther; Lete, Ester
CORPORATE SOURCE: Dep. Quimica Organica, Univ. Pais Vasco, Bilbao,
644-48080, Spain
SOURCE: Tetrahedron (1995), 51(46), 12721-30
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal

STN

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:145854

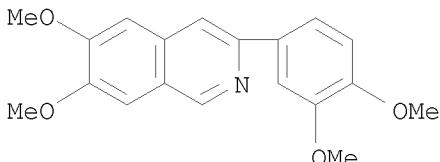
AB Several 2'-functionalized 3-arylisquinolines in different oxidation stages have been prepared. Fremy's salt or I₂/NaOAc oxidation of 2'-functionalized 3-aryltetrahydroisoquinolines always stops at the 3,4-dihydroisoquinoline stage; however, better yields and shorter reaction times are obtained with iodine. Air/KOH/DMSO oxidation of 3,4-dihydroisoquinolines furnished the aromatic derivs. with concomitant cleavage of the TBDPS group. While 3-arylisquinolin-1(2H)-ones are obtained by air oxidation of 3,4-dihydroisoquinolinium salts, the use of DDQ in dioxane resulted in a selective dehydrogenation to the corresponding N-substituted isoquinolinium salts.

IT 69504-70-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(oxidation reactions of functionalized aryltetrahydro- and
aryldihydroisoquinolines)

RN 69504-70-7 HCPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(9 CITINGS)

L13 ANSWER 62 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:862942 HCPLUS

DOCUMENT NUMBER: 124:86787

ORIGINAL REFERENCE NO.: 124:16311a, 16314a

TITLE: Acid-catalyzed cyclocondensation of nitriles. II. New synthesis of 3-aminoisoquinolines,
3-imidoylaminoisoquinolines and
3-imino-2-azaspido[4.5]deca-6,9-dien-8-one derivatives

AUTHOR(S): Sereda, A. V.; Sukhov, I. E.; Lapa, G. B.; Zolotarev, B. M.; Yartseva, I. V.; Tolkachev, O. N.

CORPORATE SOURCE: VNII Lekar. Arom. Rast., Russia

SOURCE: Zhurnal Organicheskoi Khimii (1994), 30(12), 1782-90

CODEN: ZORKAE; ISSN: 0514-7492

PUBLISHER: Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

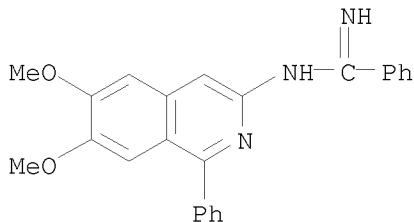
OTHER SOURCE(S): CASREACT 124:86787

AB The direction of the acid-catalyzed cyclocondensation of arylacetonitriles in presence of HCl depends on the position of the electron donor substituent in the aromatic ring of the nitrile. With the presence of one of the substituents in the 3 position electrophilic attack of the nitrile or carbonyl ion occurs at the C6 atom with the formation of substituted 3-aminoisoquinolines and the corresponding 3-imidoylaminoisoquinolines. With the use of various nitriles in the reaction mixture cocondensation

STN

occurs with the formation of a mixture of variously substituted 3-aminoisoquinolines and the corresponding amides. 4-Methoxyphenylacetonitrile and 2-bromo-4,5-dimethoxyphenylacetonitrile underwent acid-catalyzed cyclocondensation to 1-(4-methoxybenzylidene)-3-imino-2-azaspiro[4.5]deca-6,9-dien-8-one and 1-(2-bromo-4,5-dimethoxybenzylidene)-6-bromo-9-methoxy-3-imino-2-azaspiro[4.5]deca-6,9-dien-8-one, resp. Diacylamides and triazenes were obtained as addition products of the cyclocondensation. Mechanisms are suggested for the cyclocondensation.

IT 172421-54-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 172421-54-4 HCAPLUS
CN Benzenecarboximidamide, N-(6,7-dimethoxy-1-phenyl-3-isoquinolinyl)-(CA INDEX NAME)



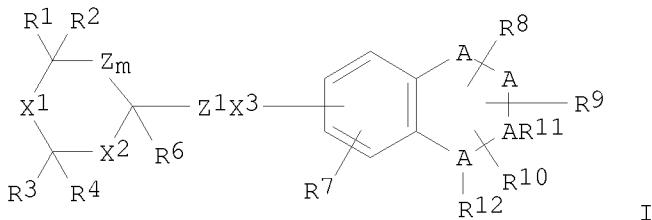
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 63 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:789143 HCAPLUS
DOCUMENT NUMBER: 123:198641
ORIGINAL REFERENCE NO.: 123:35457a,35460a
TITLE: Preparation of heteroarylquinolines as leukotriene biosynthesis inhibitors
INVENTOR(S): Friesen, Rick; Young, Robert N.; Girard, Yves; Blouin, Marc; Dube, Daniel
PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

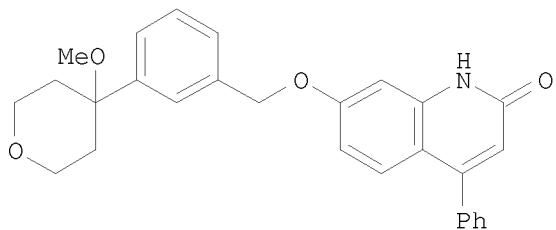
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9503300	A1	19950202	WO 1994-CA388	19940715 <--
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KE, KG, KR, KZ, LK, LT, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, TJ, TT, UA, US, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5410054	A	19950425	US 1993-95131	19930720 <--
CA 2167317	A1	19950202	CA 1994-2167317	19940715 <--

STN

AU 9472612 A 19950220 AU 1994-72612 19940715 <--
PRIORITY APPLN. INFO.: US 1993-95131 A 19930720
WO 1994-CA388 W 19940715
OTHER SOURCE(S): MARPAT 123:198641
GI



I



II

AB Title compds. [I; 1 of A = N and the others = C; Z = CHR5; R1,R5 = H, OH, alkyl, alkoxy; R2,R4 = H, alkyl; R1R2 = O; R3 = H, (hydroxy)alkyl, alkoxyalkyl; R1R3 = (oxy)alk(en)ylene; R6 = H, OH, alkyl, alkoxy, alkylthio, alkanoyloxy; R7 = H, halo, alkyl, OH, alkoxy, etc.; R8 = H, halo, CF3, alkoxy, etc.; R9,R10 = H, alkyl, heteroaryl, etc.; R11,R12 = H; R11R12 = bond; X1 = O, SOO-2, CH2; X2 = O, S, CH2, (cyclo)alkylidene; X3 = (cyclo)alkylideneoxy, -thio, etc.; Z1 = arylene; m = 0 or 1] were prepared as leukotriene biosynthesis inhibitors (no data). Thus, PhCOCH2CO2Et was amidated by 3-(MeO)C6H4NH2 and the product cyclized to give, after ether hydrolysis, 7-hydroxy-4-phenyl-2-quinolinone which was etherified by 3-(4-methoxy-4-tetrahydropyranyl)benzyl chloride to give title compound II.

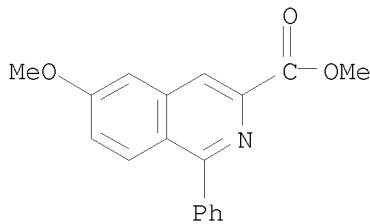
IT 167764-05-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroarylquinolines as leukotriene biosynthesis inhibitors)

RN 167764-05-8 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 6-methoxy-1-phenyl-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
 (2 CITINGS)
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 64 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1995:720049 HCAPLUS
 DOCUMENT NUMBER: 123:188478
 ORIGINAL REFERENCE NO.: 123:33241a,33244a

TITLE: Mechanism of antioxidant action of screened phenols in biological membranes. Antioxidant action of ionols "in vivo". The protective effects of lipo- and water-soluble ionol antioxidants on the cytochrome P-450 system of liver microsome membranes during lipid peroxidation

AUTHOR(S): Savov V.; Harfouf, Mahammed

CORPORATE SOURCE: Lab. Biofiz. Biomembr., Fak. Fiz., Sofia, Bulg.

SOURCE: Godishnik na Sofiiskiya Universitet "Sv. Kliment Okhridski", Fizicheski Fakultet (1995), Volume Date 1994, 86, 145-53

CODEN: GSUFA3; ISSN: 0584-0279

PUBLISHER: Universitetsko Izdatelstvo Sv. Kliment Okhridski

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The effect of ionols on the lipid peroxidn. "in vivo", induced by nonenzymic system Fe²⁺-ascorbic acid in the homogenates of rat liver and brain is studied. Relative differences in the activities of ionols are discussed. The protective effects of ionols on monooxygenase system during lipid peroxidn. in liver microsome membranes were studied. It was shown that some of these liposol. antioxidants have optimal protection effect on cytochrome P 450.

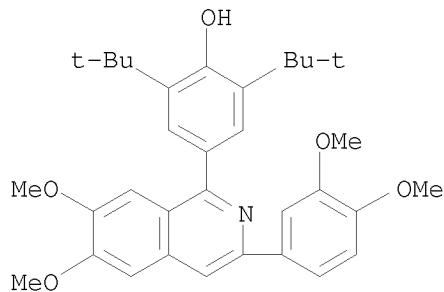
IT 132054-21-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(protective effects of lipo- and water-soluble ionol antioxidants on liver cytochrome P 450 system during lipid peroxidn.)

RN 132054-21-8 HCAPLUS

CN Phenol, 4-[3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-isoquinolinyl]-2,6-bis(1,1-dimethylethyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L13 ANSWER 65 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:621790 HCPLUS

DOCUMENT NUMBER: 123:32971

ORIGINAL REFERENCE NO.: 123:6095a

TITLE: Isoquinolines for asthma therapy

INVENTOR(S): Naef, Reto

PATENT ASSIGNEE(S): Sandoz-Patent-GmbH, Germany

SOURCE: Ger. Offen., 14 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4438737	A1	19950511	DE 1994-4438737	19941029 <--
FR 2711989	A1	19950512	FR 1994-13108	19941028 <--
FR 2711989	B1	19960614		
CH 688478	A5	19971015	CH 1994-3226	19941028 <--
GB 2283488	A	19950510	GB 1994-21985	19941101 <--
GB 2283488	B	19971203		
EP 664289	A2	19950726	EP 1994-810628	19941101 <--
EP 664289	A3	19950913		
R: BE, DK, ES, CA 2135000	GR, IE, LU, NL, PT, SE			
CA 2135000	A1	19950506	CA 1994-2135000	19941103 <--
FI 9405191	A	19950506	FI 1994-5191	19941103 <--
NO 9404187	A	19950508	NO 1994-4187	19941103 <--
AU 9477610	A	19950518	AU 1994-77610	19941103 <--
AU 685852	B2	19980129		
CZ 282329	B6	19970611	CZ 1994-2698	19941103 <--
IL 111518	A	19990620	IL 1994-111518	19941103 <--
SK 280298	B6	19991108	SK 1994-1319	19941103 <--
JP 07188176	A	19950725	JP 1994-271172	19941104 <--
CN 1106801	A	19950816	CN 1994-118199	19941104 <--
CN 1051998	C	20000503		
HU 71350	A2	19951128	HU 1994-3184	19941104 <--
HU 217120	B	19991129		
ZA 9408738	A	19960506	ZA 1994-8738	19941104 <--

STN

AT 9402048	A	19980815	AT 1994-2048	19941104 <--
AT 404940	B	19990325		
RU 2144027	C1	20000110	RU 1994-40170	19941104 <--
PL 178210	B1	20000331	PL 1994-305705	19941104 <--
US 5747506	A	19980505	US 1996-771556	19961220 <--
PRIORITY APPLN. INFO.:				
GB 1993-22828 A 19931105				
US 1994-333699 B1 19941103				
US 1995-472042 B1 19950606				
OTHER SOURCE(S):	CASREACT 123:32971; MARPAT 123:32971			
GI				

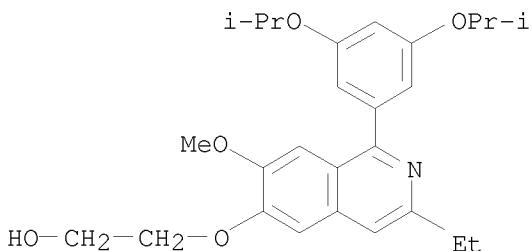
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R = Et, Pr] and their physiol. acceptable/hydrolyzable esters and/or acid addition salts are claimed. The compds. are useful for treatment of obstructive or inflammatory airway diseases, especially asthma. For example, isovanillin underwent etherification with PhCH₂OCH₂CH₂I, followed by Darzens-type condensation with EtCHBrCO₂Et and hydrolysis/decarboxylation/rearrangement of the product, to give 3-(2-benzyloxyethoxy)-4-methoxybenzyl Et ketone (II). This underwent reductive amination with NH₄OAc and NaBH₃CN, amidation of the formed amine with 3,5-diisopropoxybenzoyl chloride, and cyclization of the amide with POCl₃ in refluxing MeCN, to give dihydroquinoline derivative III. This was simultaneously dehydrogenated and hydrogenolytically deprotected by heating with 10% Pd/C in decalin at 200°, giving I (R = Et). I showed selectivity for inhibition of type IV PDE isoenzyme, and showed activity in a variety of tests, including inhibition of TNF- α secretion, inhibition of SRS-A formation, relaxation of isolated human bronchus, inhibition of chemical and biol. induced bronchoconstriction, and addnl. tests for immunosuppression.

IT 163923-99-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinolines for asthma therapy)

RN 163923-99-7 HCPLUS

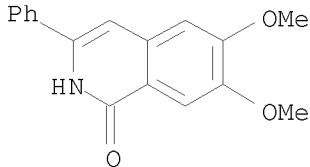
CN Ethanol, 2-[[1-[3,5-bis(1-methylethoxy)phenyl]-3-ethyl-7-methoxy-6-isoquinolinyl]oxy]- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

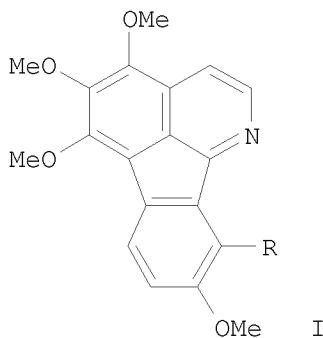
STN

L13 ANSWER 66 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:589601 HCAPLUS
DOCUMENT NUMBER: 123:169475
ORIGINAL REFERENCE NO.: 123:30251a,30254a
TITLE: Synthesis of 3-substituted isocoumarins through acyloxy palladation of o-alkenylbenzoic acids. [Erratum to document cited in CA122:132913]
AUTHOR(S): Minami, Tatsuya; Nishimoto, Akemi; Nakamura, Yumi; Hanaoka, Miyoji
CORPORATE SOURCE: Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(12), 2665
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The errors were not reflected in the abstract or the index entries.
IT 160856-44-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of substituted isocoumarins through acyloxy palladation of alkenylbenzoic acids (Erratum))
RN 160856-44-0 HCAPLUS
CN 1(2H)-Isoquinolinone, 6,7-dimethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 67 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:439791 HCAPLUS
DOCUMENT NUMBER: 122:291234
ORIGINAL REFERENCE NO.: 122:53111a,53114a
TITLE: Iminophosphorane-mediated synthesis of the carbon skeleton of the azafluoranthene alkaloids rufescine and imeluteine
AUTHOR(S): Molina, Pedro; Garcia-Zafra, Sagrario; Fresneda, Pilar M.
CORPORATE SOURCE: Fac. Quim., Univ. Murcia, Murcia, E-30071, Spain
SOURCE: Synlett (1995), (1), 43-5
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:291234
GI



AB A new four-step synthesis of the carbon skeleton of the azafluoranthenone alkaloids rufescine (I, R = H) and imeluteine (I, R = MeO) based on a aza Wittig/electrocyclic ring closure-intramolecular oxidative biaryl coupling is described.

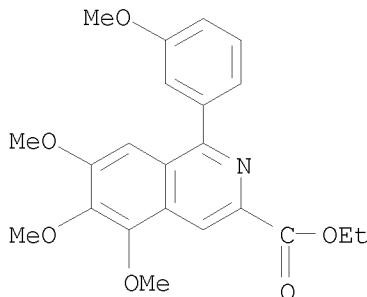
IT 163083-89-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(iminophosphorane-mediated synthesis of the carbon skeleton of the azafluoranthenone alkaloids rufescine and imeluteine)

RN 163083-89-4 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 5,6,7-trimethoxy-1-(3-methoxyphenyl)-, ethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)

L13 ANSWER 68 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:334050 HCPLUS

DOCUMENT NUMBER: 122:239509

ORIGINAL REFERENCE NO.: 122:43773a, 43776a

TITLE: Reactions of 4-(ethoxycarbonyl)benzo[c]pyrylium salts with ammonia and primary amines

AUTHOR(S): Bogza, S. L.; Zubritsky, M. Yu.; Dulenko, V. I.

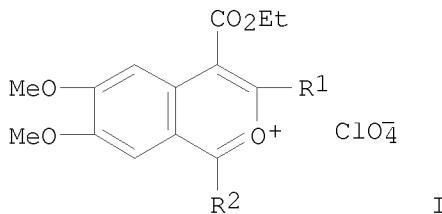
CORPORATE SOURCE: Inst. Fiz.-Org. Khim. Uglekhim., NAN Ukr., Donetsk, 340114, Ukraine

SOURCE: Khimiya Geterotsiklichesikh Soedinenii (1994), (9), 1222-4

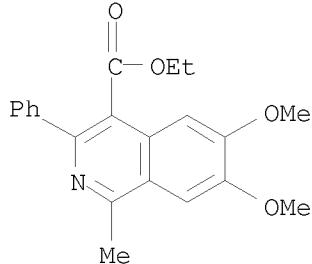
STN

PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: KGSSAQ; ISSN: 0132-6244
Latviiskii Institut Organicheskogo Sinteza
Journal
Russian



AB The title salts (I; R1 = Me, Ph; R2 = Me, Et, Pr) reacted with NH₃, BuNH₂, Me₂CHNH₂, and p-toluidine to give isoquinolines and 1-naphthylamines.
IT 162405-51-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 162405-51-8 HCPLUS
CN 4-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-methyl-3-phenyl-, ethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 69 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:334041 HCPLUS
DOCUMENT NUMBER: 122:314441
ORIGINAL REFERENCE NO.: 122:57185a, 57188a
TITLE: 2-Benzopyrylium salts. 45. Reaction of 2-benzopyrylium salts and their monocyclic analogs with ketone imines
Tosunyan, D. E.; Verin, S. V.; Kuznetsov, E. V.
Rostov. Gos. Univ., Rostov-on-Don, 344104, Russia
Khimiya Geterotsiklicheskikh Soedinenii (1994
(9), 1176-85
CODEN: KGSSAQ; ISSN: 0132-6244
PUBLISHER: Latviiskii Institut Organicheskogo Sinteza
DOCUMENT TYPE: Journal

STN

LANGUAGE: Russian

AB Ketone imines capable of imine-enamine tautomerism reacted with pyrylium salts in the enamine form. Similar reactions of 2-benzopyrylium salts gave unsatd. ketones; the monocyclic analogs gave quinolizinium or pyridinium salts.

IT 81243-45-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

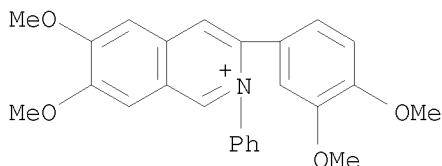
RN 81243-45-0 HCPLUS

CN Isoquinolinium, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-2-phenyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 81243-44-9

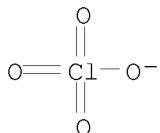
CMF C25 H24 N O4



CM 2

CRN 14797-73-0

CMF Cl O4



L13 ANSWER 70 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:296294 HCPLUS

DOCUMENT NUMBER: 122:132913

ORIGINAL REFERENCE NO.: 122:24787a, 24790a

TITLE: Synthesis of 3-substituted isocoumarins through acyloxypalladation of o-alkenylbenzoic acids

AUTHOR(S): Minami, Tatsuya; Nishimoto, Akemi; Nakamura, Yumi; Hanaoka, Miyoji

CORPORATE SOURCE: Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(8), 1700-2

CODEN: CPBTAL; ISSN: 0009-2363

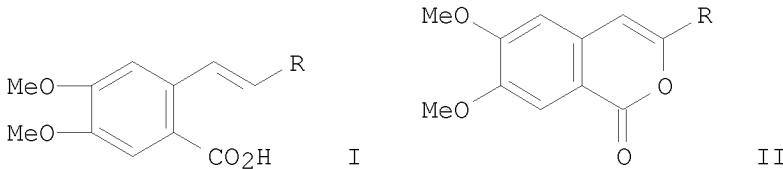
PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

STN

OTHER SOURCE(S): CASREACT 122:132913
GI



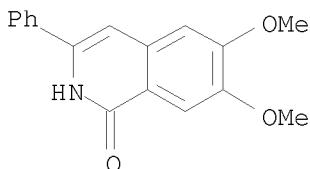
AB Cyclization of o-alkenylbenzoic acids I (Ph, substituted Ph, Bu) in the presence of Pd catalyst and benzoquinone led to 3-substituted isocoumarins II in high yield. The isocoumarins were converted to isoquinolones by treatment with primary amines.

IT 160856-44-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of substituted isocoumarins through acyloxy palladation of alkenylbenzoic acids)

RN 160856-44-0 HCAPLUS

CN 1(2H)-Isoquinolinone, 6,7-dimethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

L13 ANSWER 71 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:272292 HCAPLUS

DOCUMENT NUMBER: 122:81704

ORIGINAL REFERENCE NO.: 122:15535a,15538a

TITLE: Reaction of benzocyclobutene oxides with nitriles:
synthesis of hypcumine and other 3-substituted isoquinolines

AUTHOR(S): Fitzgerald, John J.; Michael, Forrest E.; Olofson, R. A.

CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA

SOURCE: Tetrahedron Letters (1994), 35(49), 9191-4
CODEN: TELEAY; ISSN: 0040-4039

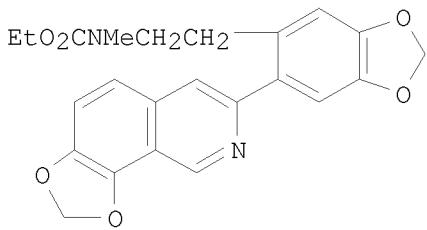
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:81704

GI



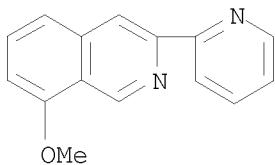
AB Treatment of benzocyclobuten-2-ols with MeLi affords o-tolualdehyde anions which in the presence of nitriles cyclize to 3-substituted isoquinolines. Examples include the synthesis of the alkaloid hypcumine (I) in 50% yield.

IT 160519-66-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of benzocyclobutene oxides with nitriles in synthesis of hypcumine and other substituted isoquinolines)

RN 160519-66-4 HCAPLUS

CN Isoquinoline, 8-methoxy-3-(2-pyridinyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L13 ANSWER 72 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:112241 HCAPLUS
DOCUMENT NUMBER: 122:31297
ORIGINAL REFERENCE NO.: 122:6175a,6178a
TITLE: The reaction of 1-aryl- and 1-pyridyl-1,2,3,4-tetrahydroisoquinolin-3-ones with dimethylcarbamoyl chloride: the preparation of amidines, isoquinolines and N-carbamoylated products
AUTHOR(S): Hunter, David J.; Markwell, Roger E.; Smith, Stephen A.; Wyman, Paul A.
CORPORATE SOURCE: Dep. Medicinal Chem., SmithKline Beecham Pharmaceuticals, Essex, CM19 5AD, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1994), (18), 2585-90
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:31297
AB 1-(Halophenyl)-1,2,3,4-tetrahydroisoquinolin-3-ones react with neat dimethylcarbamoyl chloride at 95-165°C to give high yields of the corresponding N,N-dimethylamidines; higher temps. favored

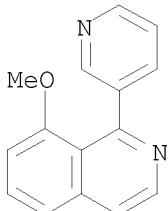
N-carbamoylation. At 155°C the related 1-(3-pyridyl)-1,2,3,4-tetrahydroisoquinolin-3-ones gave lower yields of amidine, with those lactams not bearing an electron-releasing substituent on the benzo ring gave medium to good yields of 1-(3-pyridyl)isoquinolines. In contrast, treatment of the corresponding 1-(4-pyridyl)-1,2,3,4-tetrahydroisoquinolin-3-one with neat dimethylcarbamoyl chloride at temps. between 125°C and reflux gave none of the corresponding amidine. At high temperature the N-carbamoylated product predominated, whereas at 125°C, 3-(N,N-dimethylcarbamoyloxy)-1-(4-pyridyl)isoquinoline was the major product.

IT 159769-82-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of aryl- and pyridyltetrahydroisoquinolinones with dimethylcarbamoyl chloride)

RN 159769-82-1 HCPLUS

CN Isoquinoline, 8-methoxy-1-(3-pyridinyl)-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

L13 ANSWER 73 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:570211 HCPLUS

DOCUMENT NUMBER: 121:170211

ORIGINAL REFERENCE NO.: 121:30635a, 30638a

TITLE: Hypertrophic osteopathy in rats following chronic administration of SDZ MNS 949, an isoquinoline

Laengle, U. W.; Brueggemann, S.; Prentice, D. E.; Ettlin, R. A.; Richardson, B.; Naef, R.; Cordier, A.

Sandoz Pharma Ltd., Basel, Switz.

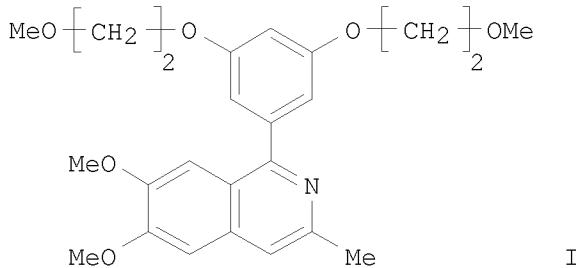
CORPORATE SOURCE: Experimental and Toxicologic Pathology (1994), 45(8), 473-9

SOURCE: CODEN: ETPAEK; ISSN: 0940-2993

DOCUMENT TYPE: Journal

LANGUAGE: English

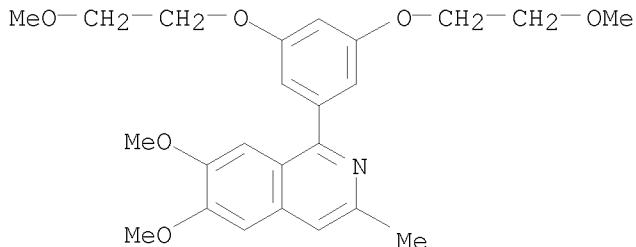
GI



AB SDZ MNS 949 (I), a bronchodilating anti-inflammatory drug that inhibits phosphodiesterase, had been proposed for the treatment of bronchial asthma. Groups of 14 male and 14 female Wistar rats were administered doses of 12, 50, and 130 mg/kg/day in feed for 26 wk. Periodic radiog. examns. were performed in addition to clin. observations, clin. chemical measurements and urinalysis. At study termination full necropsy and histopathol. examns. were performed on all animals. The principal clin. signs observed were unilateral edematous, red and painful swelling of the distal hindlimbs in 8 of 28 high dose animals, and abdominal swelling in 19 of 28 high dose animals. At radiog. examination periosteal new bone formation was predominantly along the tibia. Lesions at necropsy included dilated small and large intestines. Microscopically, enteritis was observed, and the periosteal new bone formation was confirmed. Hematol. findings consisted of thrombocytosis and lymphocytosis, especially in high dose animals. The clin., radiog. and histol. findings in treated rats were consistent with the diagnosis of "hypertrophic osteopathy" or "Marie's Disease".

IT 125175-65-7, SDZ MNS 949
 RL: BIOL (Biological study)
 (hypertrophic osteopathy from)

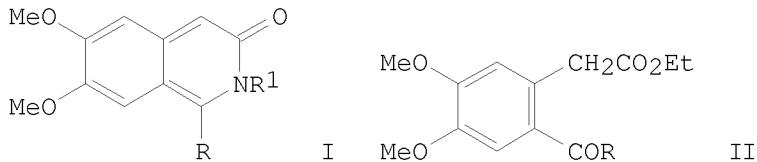
RN 125175-65-7 HCPLUS
 CN Isoquinoline, 1-[3,5-bis(2-methoxyethoxy)phenyl]-6,7-dimethoxy-3-methyl-
 (CA INDEX NAME)



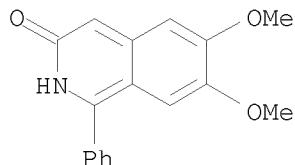
L13 ANSWER 74 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1994:435293 HCPLUS
 DOCUMENT NUMBER: 121:35293
 ORIGINAL REFERENCE NO.: 121:6511a,6514a
 TITLE: Synthesis of 3-oxo-2,3-dihydroisoquinolines from ethyl 2-acylphenylacetates and formamides
 AUTHOR(S): Venkov, A. P.; Ivanov, I. I.

STN

CORPORATE SOURCE: Dep. Chem., Univ. Plovdiv, Plovdiv, 4000, Bulg.
SOURCE: Synthetic Communications (1994), 24(8),
1145-50
CODEN: SYNCV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:35293
GI



AB Oxodihydroisoquinolines I [R = Me, Me₂CHCH₂, 3,4-(MeO)₂C₆H₃, Ph or substituted Ph, R₁ = H, Me] were obtained from acylphenylacetates II and formamides R₁NHCHO.
IT 89721-03-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 89721-03-9 HCPLUS
CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(9 CITINGS)

L13 ANSWER 75 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:269270 HCPLUS
DOCUMENT NUMBER: 120:269270
ORIGINAL REFERENCE NO.: 120:47679a, 47682a
TITLE: Structural descriptors in organic chemistry. New topological parameter based on electrotopological state of graph vertices
AUTHOR(S): Voelkel, A.
CORPORATE SOURCE: Inst. Chem. Technol. Eng., Poznan Tech. Univ., Poznan, 60-965, Pol.
SOURCE: Computers & Chemistry (Oxford, United Kingdom) (1994), 18(1), 1-4
CODEN: COCHDK; ISSN: 0097-8485
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The new topol. parameter TIE is proposed for encoding the organic structure

STN

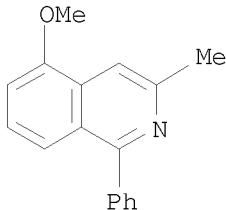
into numerical value. The discriminating power of the E-state topol. parameter TIE is discussed for the group of isoquinoline derivs.

IT 78451-50-0, Isoquinoline, 5-methoxy-3-methyl-1-phenyl-

RL: PRP (Properties)
(topol. parameter TIE of, calcn. of)

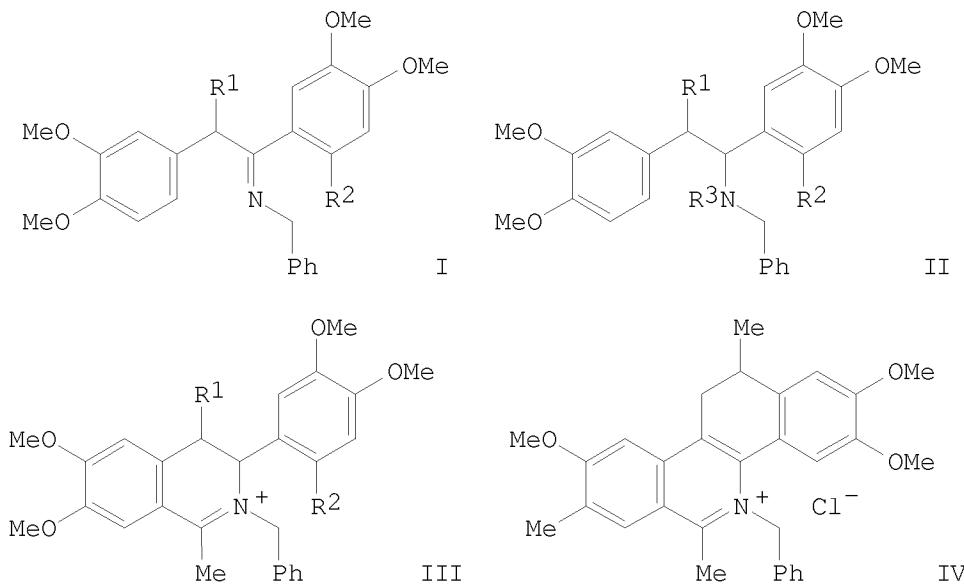
RN 78451-50-0 HCAPLUS

CN Isoquinoline, 5-methoxy-3-methyl-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L13 ANSWER 76 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:244612 HCAPLUS
DOCUMENT NUMBER: 120:244612
ORIGINAL REFERENCE NO.: 120:43349a, 43352a
TITLE: An improved method for the generation of imines and enamides. Application to the synthesis of 3-arylisoquinoline derivatives
AUTHOR(S): Sotomayor, Nuria; Vicente, Teresa; Dominguez, Esther; Lete, Esther; Villa Maria Jesus
CORPORATE SOURCE: Fac. Cienc., Univ. Pais Vasco, Bilbao, 48080, Spain
SOURCE: Tetrahedron (1994), 50(7), 2207-18
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:244612
GI



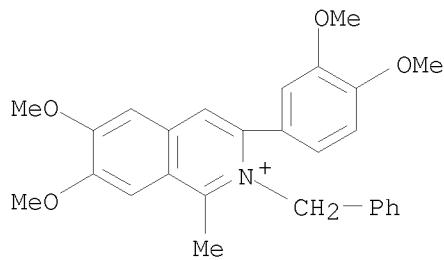
AB The one-pot preparation of hindered 1,2-diarylethylamines was achieved via Na cyanoborohydride reduction and acylation of a deoxybenzoin imine. A new methodol. for the preparation of 3-arylisoquinolinium salts by the Bischler-Napieralski reaction of 1,2-diarylethyleneamides and their transformation into 12-Me substituted benzo[c]phenanthridines was developed. Treatment of the deoxybenzoin imines I ($R_1 = H, Me, Et$; $R_2 = H, alkyl$) with benzylamine/TiCl₄/Et₃N/DME gave the amines II ($R_1 = H, Me, Et$; $R_2 = H, alkyl$; $R_3 = H$). Bischler-Napieralski reaction of the corresponding amides II ($R_1 = H, Me, Et$; $R_2 = H, alkyl$; $R_3 = acetyl$) gave isoquinolinium compds. III. From III ($R_1 = allyl$, $R_2 = H$) the benzo[c]phenanthridine IV was prepared

IT 154390-59-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 154390-59-7 HCPLUS

CN Isoquinolinium, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-2-(phenylmethyl)-, chloride (1:1) (CA INDEX NAME)

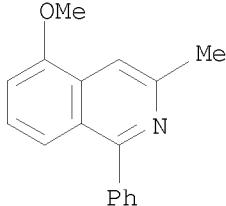


● Cl⁻

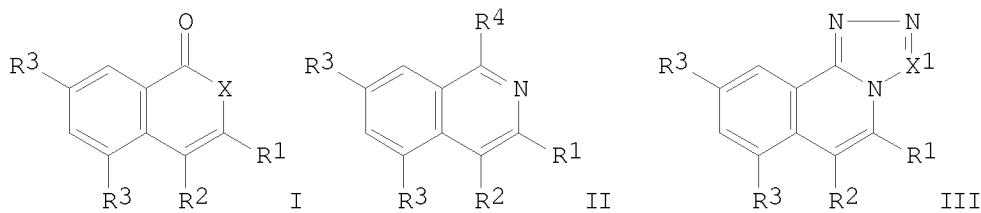
STN

OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

L13 ANSWER 77 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:133674 HCAPLUS
DOCUMENT NUMBER: 120:133674
ORIGINAL REFERENCE NO.: 120:23523a,23526a
TITLE: Structural descriptors in organic chemistry. Influence of the structure of isoquinoline derivatives upon their basicity
AUTHOR(S): Kopczynski, T.; Voelkel, A.
CORPORATE SOURCE: Inst. Chem. Technol. Eng., Poznan Tech. Univ., Poznan, 60-965, Pol.
SOURCE: THEOCHEM (1993), 103(1-2), 143-6
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Several topol. indexes were used as structural parameters in quant. structure-activity relationships for the isoquinoline derivs. Significant correlations were found between the basicity of the examined isoquinolines and their Balaban index and Wiener number
IT 78451-50-0
RL: PRP (Properties)
(influence of structure on basicity of isoquinolines)
RN 78451-50-0 HCAPLUS
CN Isoquinoline, 5-methoxy-3-methyl-1-phenyl- (CA INDEX NAME)



L13 ANSWER 78 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:649888 HCAPLUS
DOCUMENT NUMBER: 119:249888
ORIGINAL REFERENCE NO.: 119:44585a, 44588a
TITLE: Synthesis of some triazolo- and tetrazoloisoquinolines
AUTHOR(S): Bhide, B. H.; Akolkar, V. D.; Brahmbhatt, D. I.
CORPORATE SOURCE: Dep. Chem., Sardar Patel Univ., Vallabh Vidyanagar, 388 120, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1993), 32B(6), 675-8
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:249888
GI



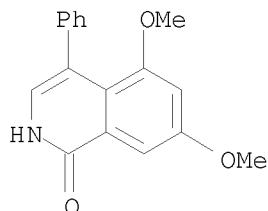
AB Treatment of isocoumarins I ($X = O$, $R1 = H$, Me , $R2 = H$, Ph , $R3 = H$, OH , OMe) with ammonia-ethanol gives isoquinolones I ($X = NH$), which react with $POCl_3-PCl_5$ affording 1-chloroisoquinolines II ($R4 = Cl$). Further reaction of II ($R4 = Cl$) with N_2H_4 furnishes 1-hydrazinoisoquinolines II ($R4 = NHNH_2$), which on treatment with HCO_2H and $NaNO_2/HCl$ provide triazoloisoquinolines III ($X1 = CH$) and tetrazoloisoquinolines III ($X1 = N$).

IT 151070-20-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

RN 151070-20-1 HCPLUS

CN 1(2H)-Isoquinolinone, 5,7-dimethoxy-4-phenyl- (CA INDEX NAME)



L13 ANSWER 79 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1993:517151 HCPLUS

DOCUMENT NUMBER: 119:117151

ORIGINAL REFERENCE NO.: 119:21067a,21070a

TITLE: 2-Benzopyrylium salts. 44. Formation of 4-acyl-3,4-dihydroisoquinolinium salts in the reaction of 2-benzopyrylium salts with azomethines and cycloaddition of maleimides to products of their deprotonation - 2,3-dihydroisoquinolines

AUTHOR(S): Tosunyan, D. E.; Verin, S. V.; Kuznetsov, E. V.

CORPORATE SOURCE: Nauchno-Issled. Inst. Fiz.-Org. Khim., Rostov-on-Don, 344104, Russia

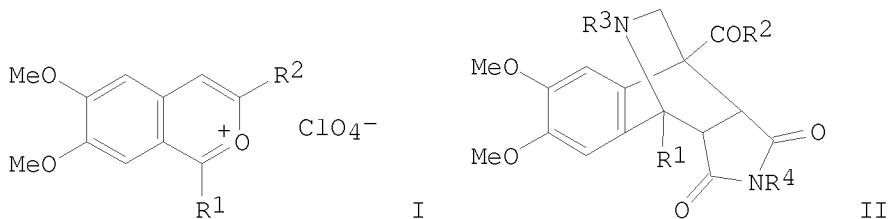
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (11), 1465-71

DOCUMENT TYPE: CODEN: KGSSAQ; ISSN: 0132-6244

LANGUAGE: Journal

OTHER SOURCE(S): Russian

GI: CASREACT 119:117151



AB The influence of substituents both in the 2-benzopyrylium cation I [R1 = H, R2 = 3,4-(MeO)2C6H3, Ph, Me] and in the azomethine PhCH:NR (R = Ph, Me) on their reactions in various solvents was confirmed. It was shown that the 4-acyl-3,4-dihydroisoquinolinium salts which are formed undergo deprotonation to give compds. with o-quinoloid structures. The last undergo cycloaddn. reactions with maleimides to give bridged salts II [R1 = H, R2 = 3,4-(MeO)C6H3, R3 = R4 = Ph, Me; R1 = H, R2-R4 = Ph].

IT 149443-04-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

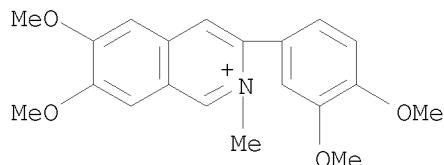
RN 149443-04-9 HCAPLUS

CN Isoquinolinium, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-2-methyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 149443-03-8

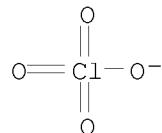
CMF C20 H22 N O4



CM 2

CRN 14797-73-0

CMF C1 O4

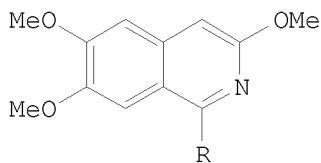


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD

STN

(1 CITINGS)

L13 ANSWER 80 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:427988 HCPLUS
DOCUMENT NUMBER: 119:27988
ORIGINAL REFERENCE NO.: 119:5185a,5188a
TITLE: A new easy one-step synthesis of isoquinoline derivatives from substituted phenylacetic esters
AUTHOR(S): Martinez, A. Garcia; Fernandez, A. Herrera; Vilchez, D. Molero; Gutierrez, M. L. Laorden; Subramanian, L. R.
CORPORATE SOURCE: Fac. Cienc. Quim., Univ. Complutense, Madrid, E-28040, Spain
SOURCE: Synlett (1993), (3), 229-30
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:27988
GI



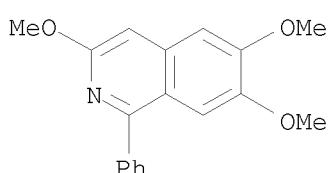
I

AB The reaction of activated phenylacetic esters, e.g., 3,4-(MeO)2C6H3CH2CO2Me, with nitriles, such as RCN (R = Me, Ph), in the presence of triflic anhydride easily affords 1-substituted 3-alkoxy isoquinolines, e.g., I, in good yields.

IT 148278-75-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 148278-75-5 HCPLUS

CN Isoquinoline, 3,6,7-trimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

L13 ANSWER 81 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:39216 HCPLUS
DOCUMENT NUMBER: 118:39216
ORIGINAL REFERENCE NO.: 118:7159a,7162a

STN

TITLE: Synthesis of the alkaloid dioxyline and other
6,7-dimethoxyisoquinolines through a modified Ritter
reaction

AUTHOR(S): Brovchenko, V. G.; Shibaeva, N. V.; Pyshchev, A. I.;
Kuznetsov, E. V.

CORPORATE SOURCE: NII Fiz. Org. Khim., Rostov-on-Don, 344006, Russia

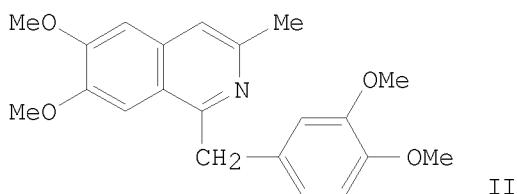
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992
(3), 363-8

DOCUMENT TYPE: CODEN: KGSSAQ; ISSN: 0132-6244
Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 118:39216

GI

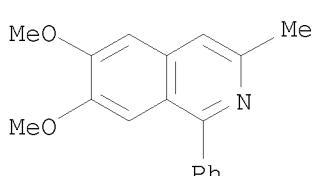


AB RCN (R = Me, Ph) and 1-(3,4-dimethoxyphenyl)-2-propanone, (I) react in the presence of acetyl perchlorate or by heating in polyphosphoric acid or in polyphosphates to give isoquinolines. The reaction proceeds via a Ritter type reaction and the conditions are determined by the electrophilic activity of the ketone carbonyl group and nucleophilicity of the nitrile. Treating I with BzCl in CH₂C₁₂ containing SbCl₅ at -90° followed by addition of 3,4-dimethoxyphenylacetonitrile gave 70% dioxyline analog II isolated as its perchlorate.

IT 20225-88-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 20225-88-1 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-3-methyl-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 82 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:651600 HCPLUS

DOCUMENT NUMBER: 117:251600

ORIGINAL REFERENCE NO.: 117:43575a, 43578a

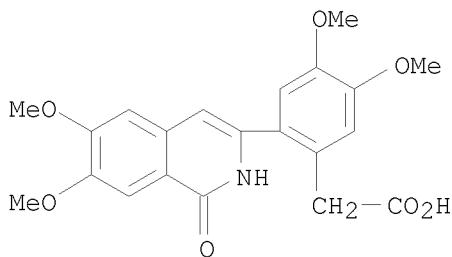
TITLE: A common and general access to berberine and

STN

AUTHOR(S): benzo[c]phenanthridine alkaloids
Beugelmans, Rene; Bois-Choussy, Michele
CORPORATE SOURCE: Inst. Chim. Subst. Nat., CNRS, Gif-sur-Yvette, 91198, Fr.
SOURCE: Tetrahedron (1992), 48(38), 8285-94
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:251600
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The SRN1 reactions between o-iodobenzamides and the enolate anion from 2-acetylhomoveratric acid lead to key tricyclic compds., e.g. I, which are easily converted to either berberine, e.g. II, or benzo[c]phenanthridine, e.g. III, ring systems providing thus a high-yielding and versatile access to both classes of alkaloids.
IT 144709-21-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 144709-21-7 HCPLUS
CN Benzeneacetic acid, 2-(1,2-dihydro-6,7-dimethoxy-1-oxo-3-isoquinolinyl)-4,5-dimethoxy- (CA INDEX NAME)

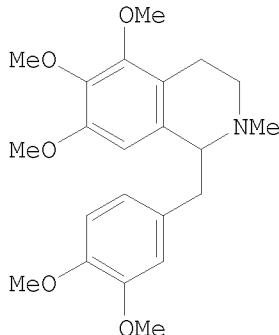


OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

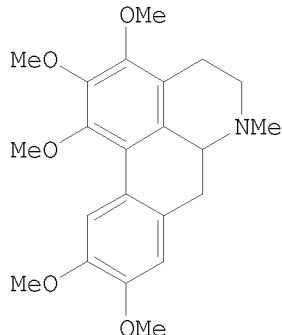
L13 ANSWER 83 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:634314 HCPLUS
DOCUMENT NUMBER: 117:234314
ORIGINAL REFERENCE NO.: 117:40543a, 40546a
TITLE: Ruthenium dioxide in fluoro acid medium. III.
Application to the synthesis of aporphinic, homoaporphinic and dibenzazocinic alkaloids. Studies towards the preparation of azafluoranthenic skeleton
Landais, Yannick; Robin, Jean Pierre
AUTHOR(S):
CORPORATE SOURCE: Dep. Chim. Inst., Univ. Technol., Le Mans, 72017, Fr.
SOURCE: Tetrahedron (1992), 48(35), 7185-96
CODEN: TETRAB; ISSN: 0040-4020

STN

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:234314
GI

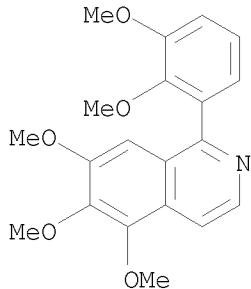


I



II

AB Intramol. oxidative couplings of phenylalkyltetrahydroisoquinoline precursors, e.g. I, in aporphinic and homoaporphinic alkaloids, e.g. II, by using RuO₂.2H₂O in fluoro acidic media were performed. A comparative study of our reagent with Tl(O₂CCF₃)₃ has been made with different precursors. The procedure was also extended to the synthesis of one dibenzoacinic alkaloid. It was attempted to synthesize the azafluoranthenic ring, using phenolic and non phenolic isoquinoline precursors.
IT 111427-25-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 111427-25-9 HCAPLUS
CN Isoquinoline, 1-(2,3-dimethoxyphenyl)-5,6,7-trimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)

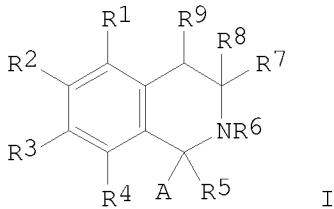
L13 ANSWER 84 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:591704 HCAPLUS
DOCUMENT NUMBER: 117:191704
ORIGINAL REFERENCE NO.: 117:33107a, 33110a
TITLE: Fungicidal isoquinoline derivatives

STN

INVENTOR(S): Bissinger, Hans Joachim; Schroeder, Ludwig; Albert, Guido; Pees, Klaus Juergen
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V., Neth.
SOURCE: Eur. Pat. Appl., 37 pp.
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 491441	A1	19920624	EP 1991-203316	19911216 <--
R: AT, BE, CH, WO 9211242	DE, DK, ES, FR, GB, GR, IT, LI, LU, NL	19920709	WO 1991-EP2444	19911216 <--
W: BR, HU, JP, KR, US				
BR 9107169	A	19931116	BR 1991-7169	19911216 <--
HU 64676	A2	19940228	HU 1993-1758	19911216 <--
JP 06503564	T	19940421	JP 1992-502072	19911216 <--
ZA 9109886	A	19920826	ZA 1991-9886	19911217 <--
PRIORITY APPLN. INFO.:			EP 1990-124372	A 19901217
			WO 1991-EP2444	A 19911216

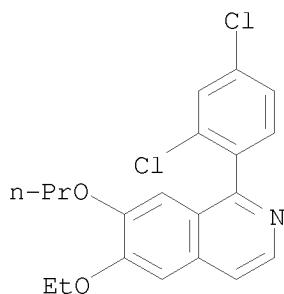
OTHER SOURCE(S): MARPAT 117:191704
GI



AB Fungicidal isoquinoline derivs. I (R1, R2, R3, R4 = H, halo, OH, alkyl, alkoxy; R1R2 or R2R3 or R3R4 together with the interjacent C atoms = 5-7-membered saturated or unsatd. carbocyclic or heterocyclic N, O, S rings; R5 = H, halo, R6 = H, R5R6 = bond; R7 = H, halo, alkyl, alkoxy, Ph, PhO, substituted Ph or PhO; R8, R9 = H or bond; A = Ph, substituted Ph) were prepared by a variety of methods. Thus, treating 3,4-(MeO)2C6H3CH2CH2NH2 with 4-PhOC6H4COCl in CH2C12 gave 88% 3,4-(MeO)2C6H3CH2CH2NHCOC6H4OPh-4 which was dehydrated by POC13 to give 66% dihydroisoquinoline II. After treatment with II cucumber-Hokus infestation with by Erysiphe cichoracearum was inhibited 11-40% after 1 wk.

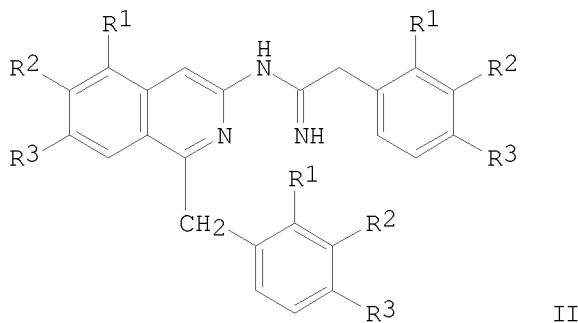
IT 143576-86-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation by chloroperoxybenzoic acid)
RN 143576-86-7 HCPLUS
CN Isoquinoline, 1-(2,4-dichlorophenyl)-6-ethoxy-7-propoxy- (CA INDEX NAME)

STN

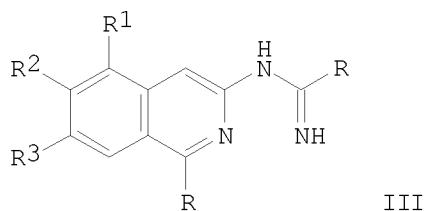


OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

L13 ANSWER 85 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:591660 HCAPLUS
DOCUMENT NUMBER: 117:191660
ORIGINAL REFERENCE NO.: 117:33099a, 33102a
TITLE: Acid promoted cyclocondensation of nitriles. I.
Novel synthesis of 3-aminoisoquinolines and their
derivatives
AUTHOR(S): Sereda, A. V.; Sukhov, I. E.; Zolotarev, B. M.;
Yartseva, I. V.; Tolkachev, O. N.
CORPORATE SOURCE: All-Union Res. Inst. Med. Plants, Moscow, 113628,
Russia
SOURCE: Tetrahedron Letters (1992), 33(29), 4205-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:191660
GI



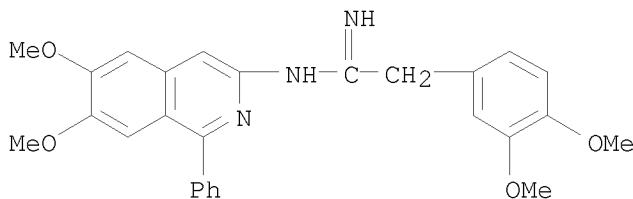
II



III

STN

AB The title reaction of nitriles R₁R₂R₃C₆H₂CN (I) gave 14-79% II (R₁ = H, R₂ = R₃ = MeO, EtO, R₂R₃ = OCH₂O; R₁ = R₂ = MeO, R₃ = H). Cyclocondensation of I with RCN gave 25.8-52.1% III (R₁, R₂, R₃ = same as above, R = Me, PhCH₂, Ph).
IT 143784-40-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 143784-40-1 HCPLUS
CN Benzeneethanimidamide, N-(6,7-dimethoxy-1-phenyl-3-isquinolinyl)-3,4-dimethoxy- (CA INDEX NAME)



L13 ANSWER 86 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:550843 HCPLUS
DOCUMENT NUMBER: 117:150843
ORIGINAL REFERENCE NO.: 117:26129a, 26132a
TITLE: Synthesis of some new 3-ethyl and 3-phenylisocoumarins
AUTHOR(S): Sinha, N. K.; Sahay, L. K.; Prasad, Kamakshya;
Srivastava, Jagdish N.
CORPORATE SOURCE: Dep. Chem., Bhagalpur Univ., Bhagalpur, 812006, India
SOURCE: Indian Journal of Heterocyclic Chemistry (1992
) , 1(5), 235-40
CODEN: IJCHEI; ISSN: 0971-1627

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Interaction of homophthalic acid I (R = Me, OMe; R₁ = OMe) with propanoic anhydride and benzoic anhydride sep. in the presence of dry pyridine at room temperature furnished isochroman-1,3-diones II (R, R₁ as above, R₂ = Et, Ph). On a steam bath temperature, the above reactions furnished 4-carboxyisocoumarins III (R, R₁, R₂ as above; R₃ = CO₂H), together with a small amount of isocoumarins III (R, R₁ as above; R₂ = 2-carboxyphenyl, R₃ = H). While condensation of I with phthalic anhydride at room temp furnished 4-carboxy-3-(2'-carboxyphenyl) isocoumarins and on a steam bath temp the above condensation afforded 3-(2'-carboxyphenyl)isocoumarins.

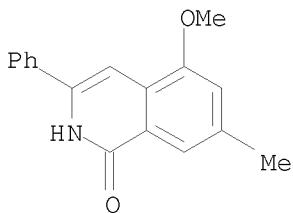
IT 143658-01-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 143658-01-9 HCPLUS

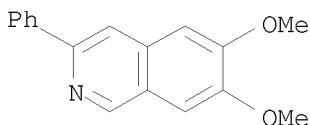
CN 1(2H)-Isoquinolinone, 5-methoxy-7-methyl-3-phenyl- (CA INDEX NAME)

STN



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L13 ANSWER 87 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:531034 HCAPLUS
DOCUMENT NUMBER: 117:131034
ORIGINAL REFERENCE NO.: 117:22747a, 22750a
TITLE: Silicon-mediated isoquinoline synthesis: preparation and stereochemical characterization of 4-hydroxy-3-phenylisoquinolines
AUTHOR(S): Badia, Dolores; Dominguez, Esther; Tellitu, Imanol
CORPORATE SOURCE: Fac. Cienc., Univ. Pais Vasco, Bilbao, 48080, Spain
SOURCE: Tetrahedron (1992), 48(21), 4419-30
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:131034
AB The silicon-mediated synthesis of 4-hydroxy-6,7-dimethoxy-3-phenylisoquinoline derivs. is reported. The described procedure implies synthetically useful yields and a high degree of stereoselectivity.
IT 24285-10-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24285-10-7 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

L13 ANSWER 88 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:511219 HCAPLUS
DOCUMENT NUMBER: 117:111219
ORIGINAL REFERENCE NO.: 117:19391a, 19394a
TITLE: Synthesis of trans-N-2-aryl(hetaryl)ethenamidines
AUTHOR(S): Nagarajan, K.; Rajagopalan, P.; Advani, B. G.; Rao, V. Ranga; Bhat, G. A.
CORPORATE SOURCE: Res. Cent., Hindustan CIBA-GEIGY Ltd., Bombay, 400 063, India
SOURCE: Proceedings - Indian Academy of Sciences, Chemical

STN

Sciences (1992), 104(3), 383-97
CODEN: PIAADM; ISSN: 0253-4134

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 117:111219

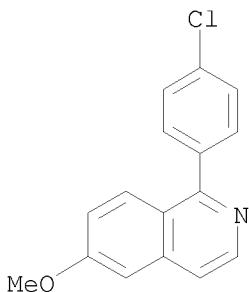
AB 2-Amino-2-arylethylamides, e.g., 3,4-(MeO)2C6H3CH(NMe2)CH2NHCOC6H4Cl-4, carrying electron-donating substituents in the para position are transformed by hot POC13 to the title compds., e.g., trans-3,4-(MeO)2C6H3CH:CHN:C(NMe2)C6H4Cl-4, presumably via iminochlorides and imidazolium derivs. Amides lacking this para substituent gave chloroamidines under these conditions.

IT 142919-84-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 142919-84-4 HCPLUS

CN Isoquinoline, 1-(4-chlorophenyl)-6-methoxy- (CA INDEX NAME)



L13 ANSWER 89 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:426284 HCPLUS

DOCUMENT NUMBER: 117:26284

ORIGINAL REFERENCE NO.: 117:4735a, 4738a

TITLE: The preparation and structural determination of 3-arylisoquinolinones

AUTHOR(S): Dominguez, Esther; Martinez de Marigorta, Eduardo;
Carrillo, Luisa; Fananas, Roberto

CORPORATE SOURCE: Fac. Cienc., Univ. Pais Vasco, Bilbao, 48080, Spain

SOURCE: Tetrahedron (1991), 47(44), 9253-8

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:26284

AB Two new methods for the oxidation of 3-aryl-3,4-dihydroisoquinolinium salts to 3-arylisoquinolinones were developed: the direct ferricyanide oxidation and the air-oxidation of 1-cyanoisoquinoline intermediates.

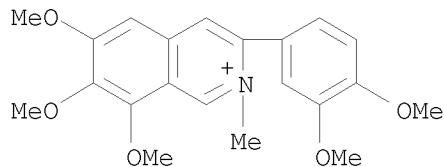
IT 138945-90-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 138945-90-1 HCPLUS

CN Isoquinolinium, 3-(3,4-dimethoxyphenyl)-6,7,8-trimethoxy-2-methyl-, iodide (1:1) (CA INDEX NAME)

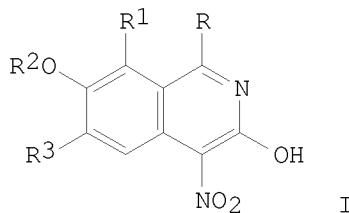
STN



● I⁻

OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L13 ANSWER 90 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:583042 HCAPLUS
DOCUMENT NUMBER: 115:183042
ORIGINAL REFERENCE NO.: 115:31253a,31256a
TITLE: Isoquinolinol derivatives: potent, short-acting inotropic and vasodilating agents with potential utility for cardiac emergencies
AUTHOR(S): Kanojia, R. M.; Press, J. B.; Lever, O. W., Jr.; Williams, L.; Werblood, H. M.; Falotico, R.; Moore, J. M.; Tobia, A. J.
CORPORATE SOURCE: Div. Med. Chem., R.W. Johnson Pharm. Res. Inst., Raritan, NJ, 08869, USA
SOURCE: European Journal of Medicinal Chemistry (1991), 26(2), 137-42
DOCUMENT TYPE: CODEN: EJMCA5; ISSN: 0223-5234
LANGUAGE: English
GI



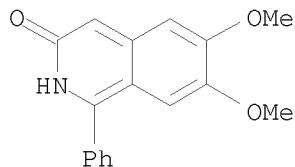
AB The title compds. I (R = H, Me, Ph; R1 = H, OMe; R2 = Me, Et, Bu; R3 = H, OMe, OEt) were prepared from the corresponding cyanides, e.g., 3,4-MeO(EtO)C₆H₃CH₂CN, via heterocyclization in HClO₄/Ac₂O and nitration. Their cardiotonic activity was studied.

IT 89721-03-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(nitration of)

RN 89721-03-9 HCAPLUS

CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)

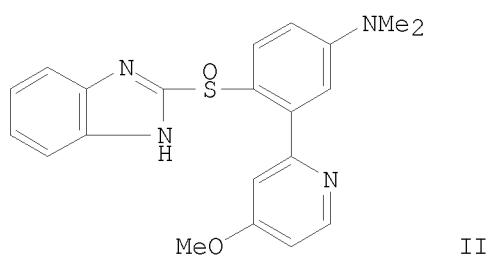
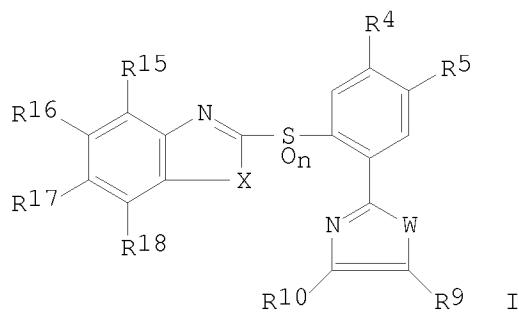
STN



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 91 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:559137 HCAPLUS
DOCUMENT NUMBER: 115:159137
ORIGINAL REFERENCE NO.: 115:27251a, 27254a
TITLE: Preparation of 2-(heteroarylphenylthio)benzimidazoles and related compounds as antiinflammatories and gastric acid secretion inhibitors
PATENT ASSIGNEE(S): Fisons PLC, UK
SOURCE: Austrian, 21 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 392788	B	19910610	AT 1988-223	19880203 <--
AT 8800223	A	19901115	AT 1988-223	19880203
PRIORITY APPLN. INFO.:			CASREACT 115:159137; MARPAT 115:159137	
OTHER SOURCE(S):				
GI				



AB Title compds. [I; X = O, NR19; W = NR8, CR7:CR8; R4,R5 = H, alkyl, alkoxy, halo, amino; R7,R8 = H, alkyl, alkoxy, amino, morpholino, (substituted) alkoxy; R9,R10 = H, alkyl; R9R10 = atoms to complete a (halo-substituted) Ph ring; R15-R18 = H, alkyl, halo, alkoxy, NO₂, amino, (modified) CO₂H; R19 = H, (substituted) alkyl; n = 0,1], were prepared as antiinflammatories and gastric acid secretion inhibitors (no data). Thus, title compound II was prepared starting from 4-O2NC6H4N2BF4 and 4-methoxypyridine N-oxide and proceeding via 2-(2-mercaptop-5-nitrophenyl)-4-methoxypyridine N,N-dimethylcarbonate.

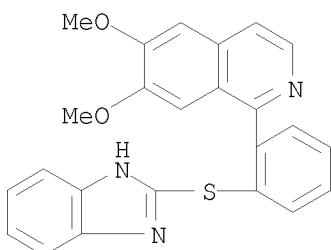
IT 115741-01-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as antiinflammatory and gastric acid secretion inhibitor)

RN 115741-01-0 HCPLUS

CN Isoquinoline, 1-[2-(1H-benzimidazol-2-ylthio)phenyl]-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

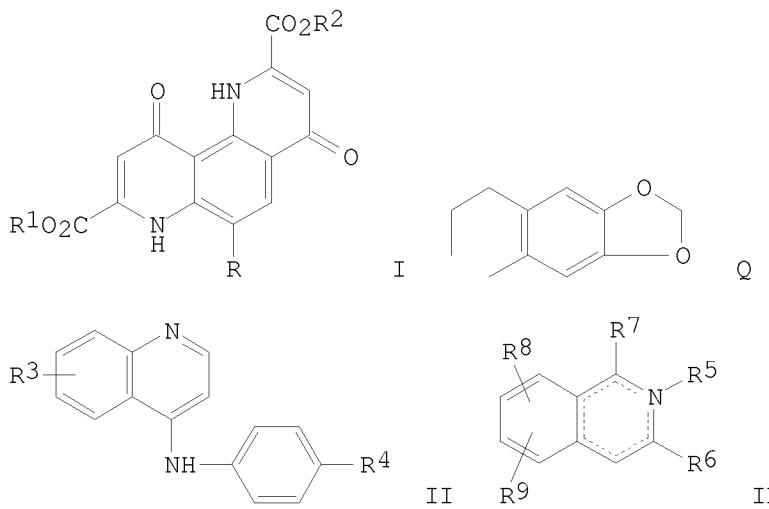
L13 ANSWER 92 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

STN

ACCESSION NUMBER: 1991:441973 HCAPLUS
DOCUMENT NUMBER: 115:41973
ORIGINAL REFERENCE NO.: 115:7121a, 7124a
TITLE: Phenanthrolinedioxodicarboxylate esters,
4-aminoquinoline, and isoquinoline derivatives as
inhibitors of HIV (human immunodeficiency virus)
reverse transcriptase
INVENTOR(S): Althaus, Irene W.; Reusser, Fritz; Tarpley, William
G.; Skaletzky, Louis L.
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: Can. Pat. Appl., 36 pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2002414	A1	19900515	CA 1989-2002414	19891107 <--
PRIORITY APPLN. INFO.:			US 1988-271567	A 19881115
			US 1988-279364	A 19881202
			US 1988-287448	A 19881220

OTHER SOURCE(S): MARPAT 115:41973
GI



AB Phenanthrolinedioxodicarboxylate esters I (R₁, R₂ = carboxyl-protecting
ester group; R = C₁₋₈ alkyl, C₅₋₆ cycloalkyl, Ph), 4-aminoquinoline
derivs. II [R₃ = halo (atomic number = 9-35), CF₃; R₄ = NHC(O)NHC₆H₅X, etc.; X
= H, halo (atomic number 9-35), CF₃, C₁₋₃ alkyloxy] etc., and isoquinoline
derivs.

STN

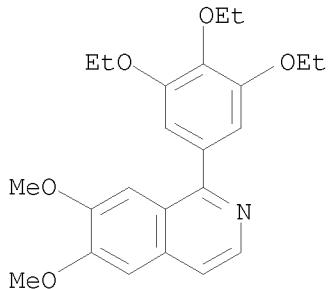
III [R6 = H or R5 and R6 = Q; R5 alone is not present; R7 = H, (CH₂)_rC₆H₃XYZ (r = 0, 1; X, Y, Z = H, C1-3 alkyloxy, C1-3 alkylcarbonyl), NHC(O)C(O)W (W = C1-3 alkyl); R8, R9 = H, C1-3 alkyloxy, C1-3 alkyloxycarbonylmethoxy] or pharmaceutically acceptable salts are used to prepare a medicament for treating a human patient infected with ≥1 strain of human immunodeficiency virus (HIV). 2'-(6,7-Dimethoxy-1-isoquinolyl)methyl)-4',5'-dimethoxyacetophenone at 100 μM inhibited reverse transcriptase by 97% and at 0.26 μM inhibited rapid syncytia formation in MT-2 cells by 10%. Et (1-isoquinolyl)oxamate was prepared by reacting 1-aminoquinoline and Et oxaryl chloride. Formulations of hard gelatin capsules, tablets, and parenteral solns. are given.

IT 6775-26-4

RL: BIOL (Biological study)
(reverse transcriptase of human immunodeficiency virus inhibition with)

RN 6775-26-4 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)-, hydrochloride
(1:1) (CA INDEX NAME)



● HCl

L13 ANSWER 93 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1991:408381 HCPLUS

DOCUMENT NUMBER: 115:8381

ORIGINAL REFERENCE NO.: 115:1629a,1632a

TITLE: Streptonigrin and related compounds. 5. Synthesis and evaluation of some isoquinoline analogs

AUTHOR(S): Rao, Koppaka V.; Beach, Joseph W.

CORPORATE SOURCE: Coll. Pharm., Univ. Florida, Gainesville, FL, 32610,
USA

SOURCE: Journal of Medicinal Chemistry (1991),
34(6), 1871-9

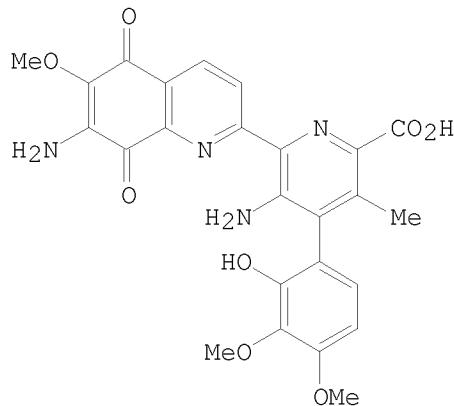
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:8381

GI



AB A series of analogs of streptonigrin (I), in which the quinoline ring is replaced by isoquinoline and the substituted pyridine is replaced by Ph, nitrophenyl, aminophenyl, or benzyl functions, have been prepared. Thus, 1-substituted isoquinoline-5,8-diones with 7-amino or 6-(alkylamino) groups were prepared. The various quinones were evaluated for antimicrobial activity against *Bacillus subtilis* and root-growth inhibitory activity against *Lepidium sativum*. The necessity of an aminoquinone function for activity is confirmed. The antibacterial activity of the isoquinoline analogs appears to be less than the quinoline derivs. However, the higher degree of antibacterial activity of the 1-benzylisoquinolines and the 1-nitrophenylisoquinolines compared to the 1-phenylisoquinolines is noteworthy. In contrast to the antibacterial activity, most of the isoquinoline analogs showed comparable or higher activity than, that of streptonigrin in a root-growth inhibition assay. The 1-nitrophenyl isoquinolines again appear to be the most active. The equal or greater potency of the benzyl analog in comparison with the Ph analog was unexpected and questions the need for the extended conjugation and the geometry required for metal binding as considered earlier.

IT 133700-36-4P

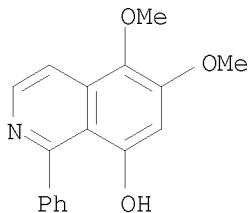
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and bromination of)

RN 133700-36-4 HCAPLUS

CN 8-Isoquinolinol, 5,6-dimethoxy-1-phenyl- (CA INDEX NAME)

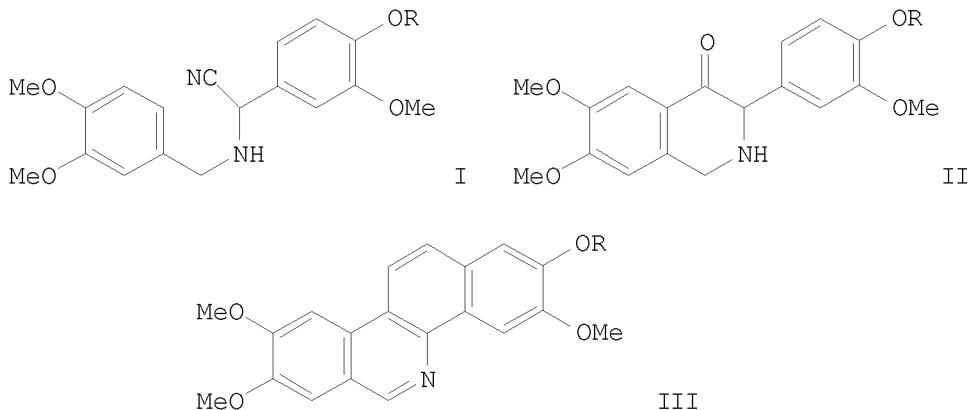


OS.CITING REF COUNT:

20

THERE ARE 20 CAPLUS RECORDS THAT CITE THIS
RECORD (20 CITINGS)

L13 ANSWER 94 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1991:102490 HCAPLUS
 DOCUMENT NUMBER: 114:102490
 ORIGINAL REFERENCE NO.: 114:17481a, 17484a
 TITLE: A very short route to fully aromatic 2,3,8,9- and
 2,3,8,9,12-oxygenated benzo[c]phenanthridines
 AUTHOR(S): Olugbade, Tiwalade A.; Waigh, Roger D.; Mackay, Simon
 P.
 CORPORATE SOURCE: Dep. Pharm., Univ. Manchester, Manchester, M13 9PL, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999) (1990), (10), 2657-60
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 114:102490
 GI

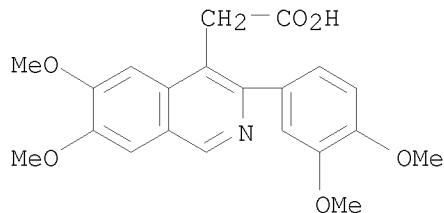


AB Cyclization of suitably substituted 2-benzylamino-2-phenylacetonitriles, I ($R = Me, Me_2CH, Et, H$), proceeds by rearrangement, in H_2SO_4 or anhydrous HF, to give 3-aryl-1,2-dihydroisoquinolinones II, possessing all but two carbons of the benzo[c]phenanthridine ring system. These two carbon atoms are introduced in high yield by a modified Reformatskii reaction and the resulting ester is cyclized in H_2SO_4 , with concomitant dehydration and oxidation, to give the fully aromatic four-ring system III in only four steps.

IT 131796-91-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclocondensation of)

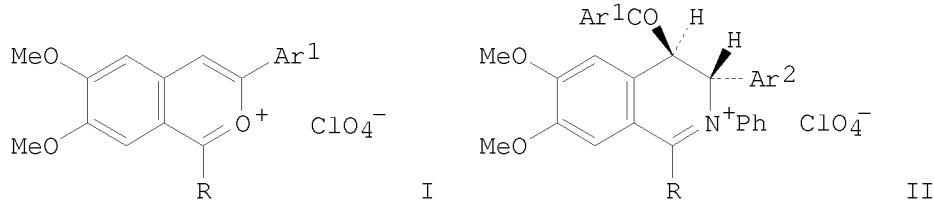
RN 131796-91-3 HCAPLUS

CN 4-Isoquinolineacetic acid, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

L13 ANSWER 95 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:100801 HCAPLUS
DOCUMENT NUMBER: 114:100801
ORIGINAL REFERENCE NO.: 114:17176h, 17177a
TITLE: 2-Benzopyrylium salts. 4. Addition of azomethines to 2-benzopyrylium salts - a new method for synthesis of isoquinolinium systems
AUTHOR(S): Verin, S.; Tosunyan, D. E.; Zakharov, P. I.; Shevtsov, V. C.; Kuznetsov, E. V.
CORPORATE SOURCE: Rostov. Gos. Univ., Rostov-on-Don, 344104, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1990), (9), 1177-80
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 114:100801
GI



AB The stereoselective recyclization reaction of benzopyrylium salts I [R = H, Ph; Ar1 = 3,4-(MeO)2C6H3] with PhN:CHAR2 (Ar2 = Ph, 4-MeOC6H4), affording trans isomers of dihydroisoquinolinium salts (II) in quant. yield, was consistent with a consecutive 1,4-cycloaddn. and onium-ring cleavage mechanism.

IT 132145-16-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

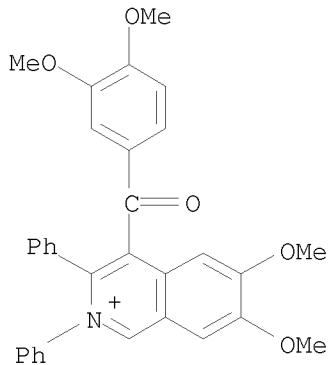
RN 132145-16-5 HCAPLUS

CN Isoquinolinium, 4-(3,4-dimethoxybenzoyl)-6,7-dimethoxy-2,3-diphenyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

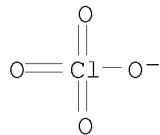
STN

CRN 132145-15-4
CMF C32 H28 N 05



CM 2

CRN 14797-73-0
CMF Cl O4

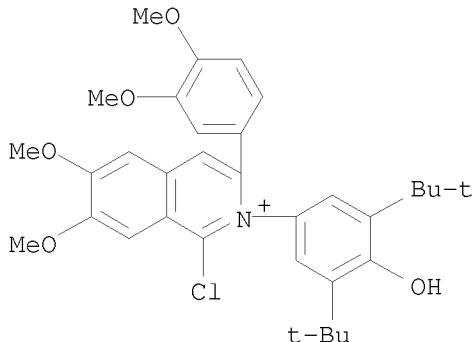


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 96 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:74727 HCPLUS
DOCUMENT NUMBER: 114:74727
ORIGINAL REFERENCE NO.: 114:12539a,12542a
TITLE: Mechanisms of antioxidant effects of shielded phenols
in biological membranes. Effects of
4-methyl-2,6-ditertbutylphenol (ionol) and its
derivatives.
AUTHOR(S): Serbinova, E.; Kharfuf, M.; Ukhin, L. Yu.; Komissarov,
V. P.; Erin, A. N.; Rakovski, S.; Savov, V.; Kagan, V.
E.
CORPORATE SOURCE: Inst. Physiol., Sofia, 1133, Bulg.
SOURCE: Byulleten Eksperimental'noi Biologii i Meditsiny (1990), 110(11), 486-9
CODEN: BEBMAE; ISSN: 0365-9615
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The antioxidant properties of ionol and 15 of its derivs. were studied in
vitro in microsomal prepns. from the rat liver. Structure-activity
relations were evaluated in lipid peroxidn. tests using Fe²⁺-NADPH and

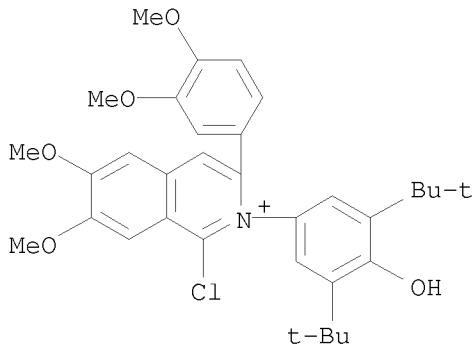
STN

Fe²⁺-ascorbate systems.
IT 132030-13-8
RL: PRP (Properties)
(antioxidant effects of, in biol. membranes, structure in relation to)
RN 132030-13-8 HCPLUS
CN Isoquinolinium, 2-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-chloro-3-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 97 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:74726 HCPLUS
DOCUMENT NUMBER: 114:74726
ORIGINAL REFERENCE NO.: 114:12539a,12542a
TITLE: Mechanisms of antioxidant effects of shielded phenols in biological membranes. Effects of 4-methyl-2,6-ditertbutylphenol (ionol) on luminol-dependent chemiluminescence
AUTHOR(S): Kharfur, M.; Serbinova, E. A.; Bakalova, R. A.; Savov, V. M.; Kagan, V. E.
CORPORATE SOURCE: Inst. Fiziolog., Sofia, 1113, Bulg.
SOURCE: Byulleten Eksperimental'noi Biologii i Meditsiny (1990), 110(11), 480-3
CODEN: BEBMAE; ISSN: 0365-9615
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The antioxidant properties of ionol and 15 of its derivs. were studies in vitro in rat liver microsomal preps. The incubation media contained Fe²⁺-NADPH or Fe²⁺-ascorbate, luminol, and K₂O₂. Luminol-dependent chemiluminescence was measured as an index of lipid peroxidn. The concurrent effects of catalase and superoxide dismutase were also evaluated. The data were related to structural aspects (lipophilicity and heptane/water partition) of the antioxidants.
IT 132030-13-8
RL: PRP (Properties)
(antioxidant effects of, structure in relation to)
RN 132030-13-8 HCPLUS
CN Isoquinolinium, 2-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-chloro-3-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



L13 ANSWER 98 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1991:30144 HCPLUS

DOCUMENT NUMBER: 114:30144

ORIGINAL REFERENCE NO.: 114:5187a, 5190a

TITLE: Pharmaceutical compounds active on presbyopia,
comprising ganglioplegics and spasmolytics

INVENTOR(S): Corbiere, Jerome

PATENT ASSIGNEE(S): Fr.

SOURCE: Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 369880	A1	19900523	EP 1989-403141	19891115 <--
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE FR 2638970	A1	19900518	FR 1988-14907	19881116 <--
PRIORITY APPLN. INFO.:			FR 1988-14907	A 19881116

AB Drug compns. for the treatment of presbyopia comprise a spasmolytic or a ganglioplegic agent (no data). Both agents are of the musculotropic type. The spasmolytics are phenolic or quaternary ammonium compds. The ganglioplegics are papaverine, ethaverine, octaverine, enkephalinergic agonists, butyrophenones, etc. A collyrium comprised pinaverium bromide 1, NaH₂PO₄.2H₂O 1, Na₂HPO₄.12H₂O 9.38 g, benzalkonium chloride 18.48 mg, Na hypophosphite 0.1 g, and water to 1 L.

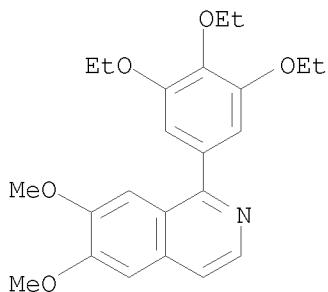
IT 549-68-8, Octaverine

RL: BIOL (Biological study)
(collyrium for presbyopia treatment containing)

RN 549-68-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)

STN



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 99 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:612013 HCAPLUS
DOCUMENT NUMBER: 113:212013
ORIGINAL REFERENCE NO.: 113:35835a,35838a
TITLE: Preparation of phenanthroline dicarboxylate esters,
4-aminoquinoline and isoquinoline derivatives as
inhibitors of HIV reverse transcriptase
INVENTOR(S): Althaus, Irene W.; Reusser, Fritz; Tarpley, William
Gary; Skaletzky, Louis L.
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9005523	A2	19900531	WO 1989-US4774	19891030 <--
WO 9005523	A3	19900712		
	W: AU, DK, FI, HU, JP, KR, NO, SU, US RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE			
AU 8944889	A	19900612	AU 1989-44889	19891030 <--
PRIORITY APPLN. INFO.:			US 1988-271567	A 19881115
			US 1988-279364	A 19881202
			US 1988-287448	A2 19881220
			WO 1989-US4774	A 19891030
OTHER SOURCE(S):	MARPAT	113:212013		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I, II, III, IV, etc.; R = C1-8 alkyl, C5-8 cycloalkyl, Ph; R1, R2 = CO2H-protecting ester group; R3 = N-benzoyl- or N-phenylsulfonylpiperazin-4-ylcarbonyl, NHCONHPh, or N-(4-phenylcyclohex-3-en-1-yl)carbamoyl optionally substituted on the Ph ring, morpholinocarbonyl; R4 = F, Cl, Br, CF3; X = H, F Cl, Br, CF3, Cl-3

STN

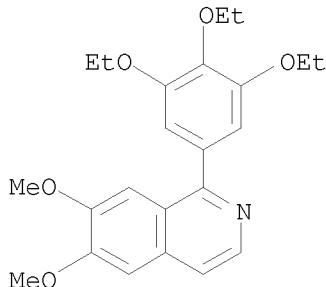
alkoxy; R5 = H, Ph or PhCH₂ optionally substituted on the Ph ring; R6, R7 = H, Cl-3 alkoxy or alkoxy carbonylmethyl] some of which are new, known, or com. available, are useful for treatment of patients afflicted with HIV. Thus, to 1-[4-[(7-trifluoromethyl-4-quinolinyl)amino]benzoyl]piperazine in the THF was added Et₃N followed by BzCl and the resulting mixture was stirred 24 h at room temperature to give 1-benzoyl-4-[4-[(7-trifluoromethyl-4-quinolinyl)amino]benzoyl]piperazine. A total of 16 I were prepared and 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)isoquinoline HCl (octaverine HCl) (V) inhibited 70% at 2.30 μM HIV-induced syncytia formation in a tissue culture of MT-2 cells. Tablets containing V and 8 other pharmaceutical compns. containing 7 specific I were formulated.

IT 6775-26-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as HIV reverse transcriptase inhibitor)

RN 6775-26-4 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)-, hydrochloride
(1:1) (CA INDEX NAME)



● HCl

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 100 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:571360 HCPLUS
DOCUMENT NUMBER: 113:171360
ORIGINAL REFERENCE NO.: 113:29057a,29060a
TITLE: Studies on the ultraviolet spectra of
3(2H)-isoquinolinones and their saturated derivatives
AUTHOR(S): Hazai, Laszlo; Deak, Gyula; Hazai-Horvath, Judit;
Toth, Gabor
CORPORATE SOURCE: Inst. Exp. Med., Hung. Acad. Sci., Budapest, H-1450,
Hung.
SOURCE: Acta Chimica Hungarica (1989), 126(6),
869-78
CODEN: ACHUDC; ISSN: 0231-3146
DOCUMENT TYPE: Journal
LANGUAGE: English

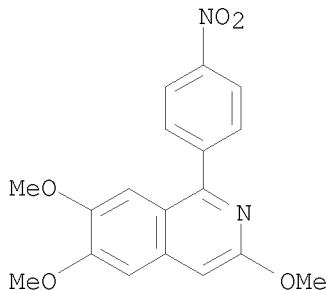
STN

AB The UV spectral data of some newly synthesized 3(2H)-isoquinolinones and their derivs. are given. The characteristic bands in the UV spectra of 5,6,7,8-tetrahydro- and 1,4-dihydro-3(2H)-isoquinolinones are also surveyed and compared with the spectra of derivs. having fixed lactam or lactim structure to establish the probable tautomeric forms. Relevant literature data are used for comparison in presenting the UV spectra of 3-chloro- and 3-amino-5,6,7,8-tetrahydroisoquinolines.

IT 129975-08-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 129975-08-2 HCPLUS

CN Isoquinoline, 3,6,7-trimethoxy-1-(4-nitrophenyl)- (CA INDEX NAME)

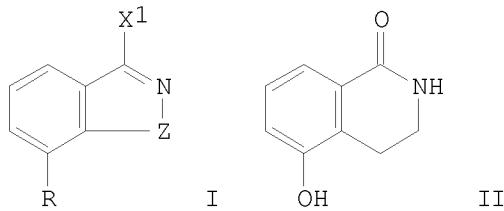


L13 ANSWER 101 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:532025 HCPLUS
DOCUMENT NUMBER: 113:132025
ORIGINAL REFERENCE NO.: 113:22427a,22430a
TITLE: Preparation of substituted dihydroisoquinolinones and related compounds as radiation therapy potentiators and chemotherapeutic agents
INVENTOR(S): Suto, Mark James; Turner, William Richard; Werbel, Leslie Morton
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: Eur. Pat. Appl., 32 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 355750	A1	19900228	EP 1989-115300	19890818 <--
EP 355750	B1	19950125		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 02124874	A	19900514	JP 1989-211506	19890818 <--
JP 2786896	B2	19980813		
CA 1334969	C	19950328	CA 1989-608774	19890818 <--
ES 2067508	T3	19950401	ES 1989-115300	19890818 <--
US 5177075	A	19930105	US 1991-758180	19910911 <--
PRIORITY APPLN. INFO.:			US 1988-234704	A 19880819
			US 1989-372751	A 19890703

STN

OTHER SOURCE(S): MARPAT 113:132025
GI



AB The title compds. [I; R = alkyl, halo, NC, F3C, R1O, R1R2N, X2CO, X2O2C, R1 = H, alkyl, PhCH₂, (CH₂)_nCH(OH)_y(CH₂)_mA; R2 = H, alkyl, Ph, PhCH₂; X2 = alkyl, aryl, aralkyl; m = 0-5, n = 1-4; y = 0, 1; A = R2O, Me₂N, Et₂N, Ph, morpholino, piperidino, pyrrolidino; X1 = R1O, S(C1-4 alkyl), R4R5N, R4, R5 = H, alkyl, PhCH₂, alkanoyl, (CH₂)_n(CHOH)_y(CH₂)_mQ, Q = Me₂N, Et₂N; Z = CHR₂CHR₃, R3 = H, alkyl, Ph, PhCH₂, etc.], their stereoisomers, mixts., and salts, enhancers of the lethal effects for tumor cells by ionizing radiation or chemotherapy, were prepared 1,5-Dihydroxyisoquinoline in AcOH containing Pd/C was hydrogenated at room temperature to give the isoquinolinone II.

In vivo II showed a radiosensitizing activity comparable to misonidazole.

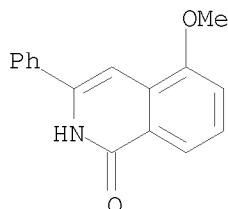
IT 129075-63-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as sensitizer to chemotherapeutic- and radiation agents)

RN 129075-63-4 HCPLUS

CN 1(2H)-Isoquinolinone, 5-methoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 37 THERE ARE 37 CAPLUS RECORDS THAT CITE THIS RECORD (46 CITINGS)

L13 ANSWER 102 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:497871 HCPLUS
DOCUMENT NUMBER: 113:97871
ORIGINAL REFERENCE NO.: 113:16545a,16548a
TITLE: A novel base-catalyzed carbon-nitrogen bond fission in some heterocycles
AUTHOR(S): Lal, Banshi; Gidwani, Ramesh M.; De Souza, Noel J.
CORPORATE SOURCE: Hoechst Cent. Basic Res., Hoechst India Ltd., Mulund, 400 080, India
SOURCE: Journal of Organic Chemistry (1990), 55(17), 5117-24

STN

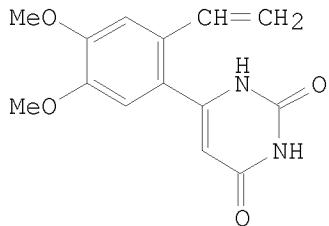
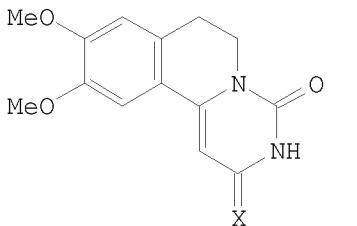
DOCUMENT TYPE:
LANGUAGE:
OTHER SOURCE(S):
GI

CODEN: JOCEAH; ISSN: 0022-3263

Journal

English

CASREACT 113:97871



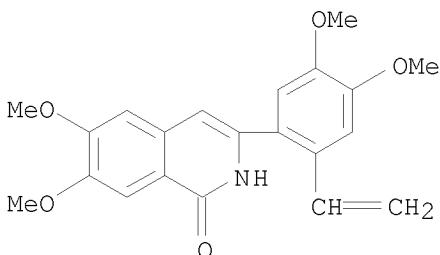
AB N heterocycles bearing a nonbasic N atom and other defined structural features as exemplified by 9,10-dimethoxy-3,4,6,7-tetrahydro-2H-pyrimido[6,1-a]isoquinoline-2,4-dione (I), 8-oxypseudopalmatine, 8-oxypseudoberberine, rutaecarpine, and related systems, on heating with excess NaH in polar aprotic solvents, undergo a facile C-N bond cleavage reaction to give new N heterocycles with an arylvinyl group as one of the substituents. The nature, scope, postulated mechanism, and limitations of this novel C-N bond cleavage reaction are described. Thus, cleavage of I with NaH in DMF gave vinyl derivative 50% II.

IT 60315-12-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 60315-12-0 HCAPLUS

CN 1(2H)-Isoquinolinone, 3-(2-ethenyl-4,5-dimethoxyphenyl)-6,7-dimethoxy-
(CA INDEX NAME)



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L13 ANSWER 103 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:405606 HCAPLUS

DOCUMENT NUMBER: 113:5606

ORIGINAL REFERENCE NO.: 113:1091a,1094a

TITLE: Basicity of 1,3-disubstituted isoquinolines

AUTHOR(S): Zielinski, Wojciech

STN

CORPORATE SOURCE: Inst. Org. Chem. Technol., Silesian Polytech. Univ.,
Gliwice, 44101, Pol.

SOURCE: Polish Journal of Chemistry (1989), 63(1-3),
233-7

CODEN: PJCHDQ; ISSN: 0137-5083

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Values of pKa for 1,3-dimethylisoquinoline, 1-phenyl-3-methylisoquinoline and a series of their 5, 6 and 7-substituted derivs. were determined in 50% volume/volume aqueous methanol solution by the spectrophotometric method. The determined

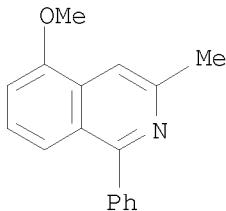
values of pKa were correlated with the Hammett σ consts. Good correlations were obtained for 5 and 7-substituted derivs. with σ_m consts. and for 6-substituted derivs. with σ_p consts. The electronic effects occurring in the isoquinoline system under study are discussed.

IT 78451-50-0, 5-Methoxy-3-methyl-1-phenylisoquinoline

RL: PRP (Properties)
(basicity of)

RN 78451-50-0 HCAPLUS

CN Isoquinoline, 5-methoxy-3-methyl-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 104 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:216661 HCAPLUS

DOCUMENT NUMBER: 112:216661

ORIGINAL REFERENCE NO.: 112:36569a, 36572a

TITLE: An unexpected access to
1-(trifluoromethyl)isoquinolines,
4-hydroxy-1-(trifluoromethyl)isoquinolines and
8a-(trifluoromethyl)cycloheptatrieno[b]pyrroles from
5-benzyloxy-4-(trifluoromethyl)oxazoles

AUTHOR(S): Burger, Klaus; Schierlinger, Christian; Gaa, Karl;
Geith, Klaus; Sewald, Norbert; Mueller, Gerhard

CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Muenchen, Garching,
D-8046, Fed. Rep. Ger.

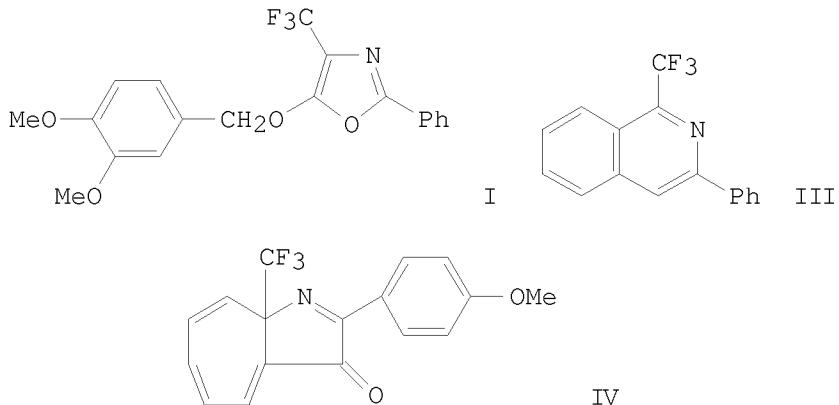
SOURCE: Chemiker-Zeitung (1989), 113(9), 277-81
CODEN: CMKZAT; ISSN: 0009-2894

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 112:216661

GI



AB 5-Benzyl-4-(trifluoromethyl)oxazoles, e.g. I, are thermolabile compds. They rearrange to give 4-benzyl-4-trifluoromethyl-5(4H)-oxazolones and/or 2-benzyl-4-trifluoromethyl-5(2H)-oxazolones (II) in some cases already at room temperature in the crystalline state. The rearrangement involves a benzyl group

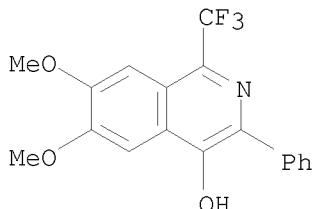
migration from O to C. Mixed products in crossing expts. indicate that the rearrangement is not a sigmatropic process. II on thermolysis undergo a [3 + 2] cycloreversion process to give nitrile ylides, which react as 1,3-dipoles or as carbenes, depending on the substituent pattern present at the benzylic moiety, to give 1-trifluoromethylisoquinolines, e.g. III, 4-hydroxy-1-trifluoromethylisoquinolines, and 8a-trifluoromethylcycloheptatrieno[b]pyrroles, e.g. IV.

IT 127029-60-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 127029-60-1 HCAPLUS

CN 4-Isoquinolinol, 6,7-dimethoxy-3-phenyl-1-(trifluoromethyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L13 ANSWER 105 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

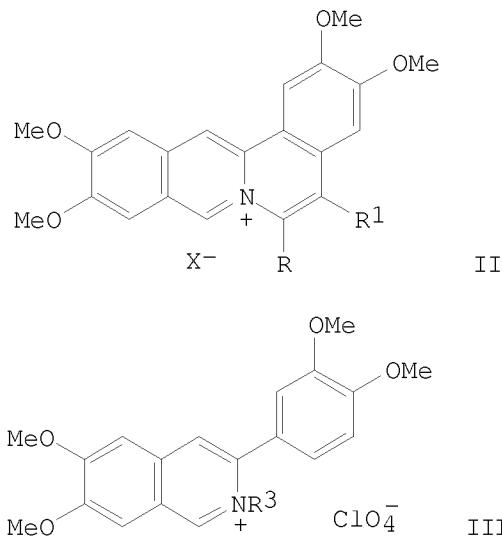
ACCESSION NUMBER: 1990:179554 HCAPLUS

DOCUMENT NUMBER: 112:179554

ORIGINAL REFERENCE NO.: 112:30385a, 30388a

TITLE: 2-Benzopyriliun salts. 35. Synthesis of the natural

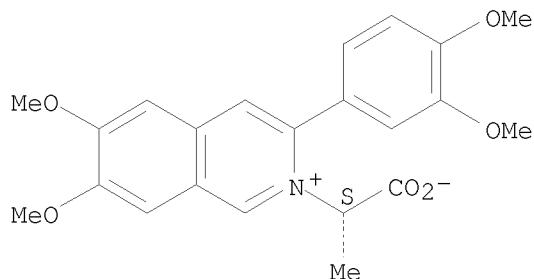
AUTHOR(S): alkaloid dehydronorcoralydine and other substituted salts of dibenzo[a,g]quinolizine
 CORPORATE SOURCE: Shcherbakova, I. V.; Verin, S. V.; Kuznetsov, E. V.
 Nauchno-Issled. Inst. Fiz.-Org. Khim., Rostov. Gos.
 Univ., Rostov-on-Don, USSR
 SOURCE: Khimiya Prirodnikh Soedinenii (1989), (1),
 75-80
 DOCUMENT TYPE: CODEN: KPSUAR; ISSN: 0023-1150
 Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 112:179554
 GI



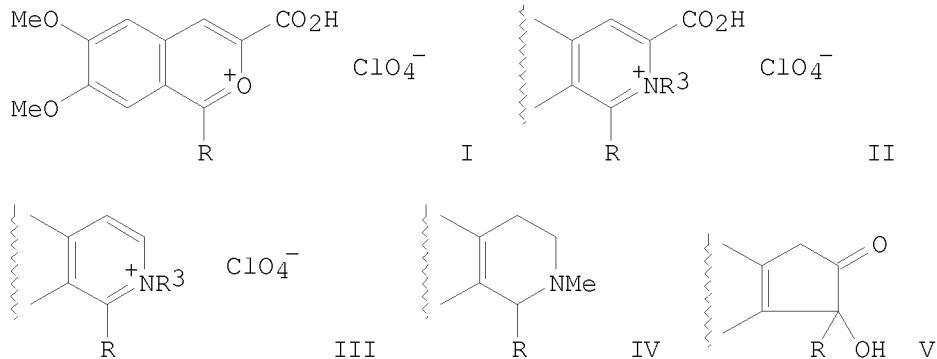
AB *6,7-Dimethoxy-3-(3,4-dimethoxyphenyl)-2-benzopyrylium perchlorate (I) recyclized with H₂NCH₂CH(OEt)₂ in refluxing EtOAc to give 70% title alkaloid (II; R = R₁ = H, X = Cl). Analogous reaction of I with H₂NCHR₂CO₂H (R₂ = H, Me) gave 50% N-ethylisoquinolinium salt III (R₃ = Et) in BuOH and 70-85% III (R₃ = CHR₂CO₂-; same R₂; no counterion) in EtOH or AcOH. These betaines gave 98% III (R₃ = CHR₂CO₂H; same R₂) with HClO₄ in aqueous EtOH and cyclized with polyphosphoric acid to give 60-65% II (R = same R₂; R₁ = OH), and the latter were acetylated to give the corresponding II (R₁ = OAc) in 70% yield.*

IT 126522-95-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and intramol. cyclocondensation reaction of)
 RN 126522-95-0 HCPLUS
 CN Isoquinolinium, 2-(1-carboxyethyl)-3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-, inner salt, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 106 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1990:178614 HCPLUS
 DOCUMENT NUMBER: 112:178614
 ORIGINAL REFERENCE NO.: 112:30205a, 30208a
 TITLE: 2-Benzopyrylium salts. 34. Reaction of 3-carboxy-2-benzopyrylium salts with amines; synthesis of cyclic ketones
 AUTHOR(S): Zhdanov, u. A.; Brovchenko, V. G.; Klyuev, N. A.; Kuznetsov, E. V.
 CORPORATE SOURCE: Rostov. Gos. Univ., Rostov, 344071, USSR
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1989), (4), 454-9
 CODEN: KGSSAQ; ISSN: 0453-8234
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 112:178614
 GI



AB Treating benzopyrylium perchlorate I ($R = 3,4-R_1R_2C_6H_3$; $R_1 = MeO, H$; $R_2 = MeO$) with R_3NH_2 ($R_3 = Ph, Me$) in EtOH gave 90-97% yields of the corresponding isoquinolinium perchlorates II, which were decarboxylated by piperidine in xylene to give 91-98% isoquinolinium perchlorates III (same $R-R_3$). III were reduced by $NaBH_4$ to give 85 and 89% tetrahydroisoquinolines IV. Also obtained were indanones V.

IT 126324-88-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

STN

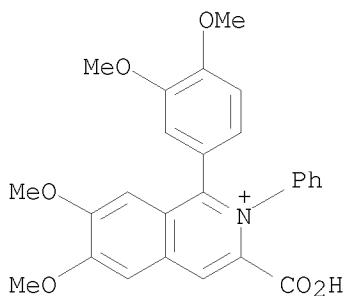
(Reactant or reagent)
(preparation and decarboxylation of)

RN 126324-88-7 HCPLUS

CN Isoquinolinium, 3-carboxy-1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-2-phenyl-, perchlorate (1:1) (CA INDEX NAME)

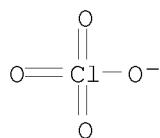
CM 1

CRN 126324-87-6
CMF C26 H24 N O6

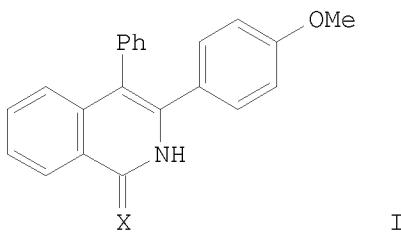


CM 2

CRN 14797-73-0
CMF Cl O4



L13 ANSWER 107 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:138890 HCPLUS
DOCUMENT NUMBER: 112:138890
ORIGINAL REFERENCE NO.: 112:23475a, 23478a
TITLE: Photolysis of vinyl halides. Reaction of photogenerated vinyl cations with cyanate and thiocyanate ions
AUTHOR(S): Kitamura, Tsugio; Kobayashi, Shinjiro; Taniguchi, Hiroshi
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Journal of Organic Chemistry (1990), 55(6), 1801-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:138890
GI



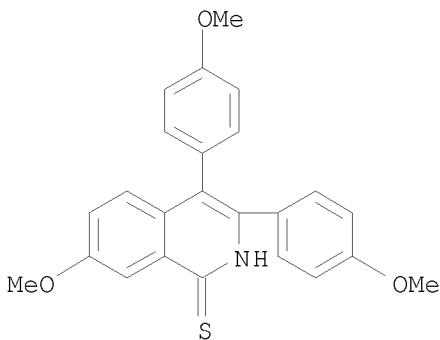
AB The title reaction was conducted in a two-phase system of CH₂Cl₂ and water using a tetrabutylammonium halide as a phase-transfer catalyst. The reaction of the photogenerated arylvinyl cations, e.g. (Ph₂C:C+C₆H₄OMe-4)Br- with cyanate ion gave only isoquinolone derivs., e.g. I (X = O), whereas the reaction with thiocyanate ion afforded products derived from S attack, vinyl thiocyanates, and products derived from N attack, vinyl isothiocyanates or isoquinolinethiones, e.g. I (X = S). The ambident nature of thiocyanate ion is compared with the reaction of benzyl bromides.

IT 93119-56-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 93119-56-3 HCPLUS

CN 1(2H)-Isoquinolinethione, 7-methoxy-3,4-bis(4-methoxyphenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)

L13 ANSWER 108 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:76968 HCPLUS

DOCUMENT NUMBER: 112:76968

ORIGINAL REFERENCE NO.: 112:13151a, 13154a

TITLE: Preparation of 1-phenylisoquinolines as bronchodilators

INVENTOR(S): Hasspacher, Klaus; Naef, Reto

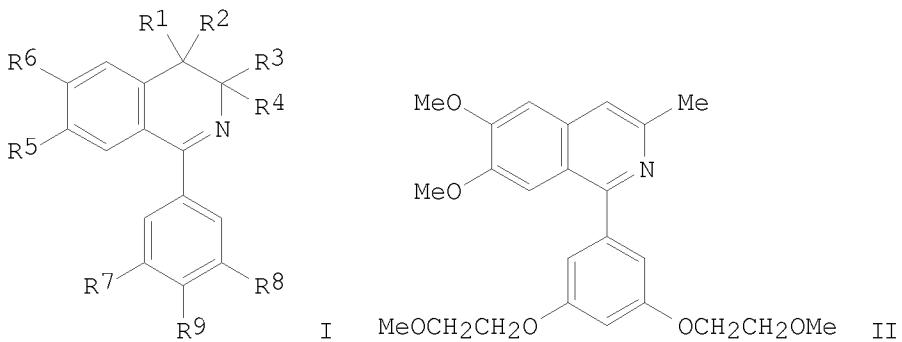
PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 13 pp.

STN

CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3900233	A1	19890720	DE 1989-3900233	19890105 <--
DE 3900233	C2	20000427		
HU 52061	A2	19900628	HU 1989-11	19890103 <--
HU 205083	B	19920330		
GB 2213482	A	19890816	GB 1989-102	19890104 <--
GB 2213482	B	19910911		
SE 8900039	A	19890709	SE 1989-39	19890105 <--
SE 501548	C2	19950313		
ES 2010071	A6	19891016	ES 1989-53	19890105 <--
CA 1332944	C	19941108	CA 1989-587599	19890105 <--
DK 8900057	A	19890709	DK 1989-57	19890106 <--
FI 8900072	A	19890709	FI 1989-72	19890106 <--
FI 90865	B	19931231		
FR 2625743	A1	19890713	FR 1989-128	19890106 <--
FR 2625743	B1	19901109		
AU 8927795	A	19890720	AU 1989-27795	19890106 <--
AU 622429	B2	19920409		
NL 8900029	A	19890801	NL 1989-29	19890106 <--
JP 01213267	A	19890828	JP 1989-1898	19890106 <--
JP 06049686	B	19940629		
ZA 8900133	A	19900926	ZA 1989-133	19890106 <--
BE 1002730	A3	19910521	BE 1989-18	19890106 <--
PL 156099	B1	19920228	PL 1989-277092	19890106 <--
IL 88899	A	19940731	IL 1989-88899	19890106 <--
AT 8900035	A	19910915	AT 1989-35	19890109 <--
AT 394365	B	19920325		
CH 678727	A5	19911031	CH 1989-59	19890109 <--
US 4980359	A	19901225	US 1990-507702	19900410 <--
			GB 1988-397	A 19880108
			US 1989-294431	B1 19890106
PRIORITY APPLN. INFO.:				
OTHER SOURCE(S):		CASREACT 112:76968; MARPAT 112:76968		
GI				



STN

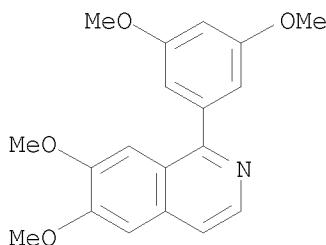
AB The title compds. (I; R₁, R₃ = H, C1-4 alkyl; R₂ = H; R₂R₃ = bond; R₄ = H, C1-4 alkyl, Ph; R₅ = MeO, EtO; R₆ = H, OH, C1-4 alkoxy, etc.; R₇, R₈ = C1-4 alkoxy, alkoxyalkoxy; R₉ = H, halo) were prepared as bronchodilators (no data). Thus, N-[3-(3,4-dimethoxyphenyl)-2-propyl]-3,5-dimethoxyethoxybenzamide was refluxed 5 h with POCl₃ in MeCN and the product was heated 5 h at 200° with Pd/C in decalin to give II obtained as oxalate.

IT 125142-32-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as bronchodilator)

RN 125142-32-7 HCPLUS

CN Isoquinoline, 1-(3,5-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 109 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:76914 HCPLUS

DOCUMENT NUMBER: 112:76914

ORIGINAL REFERENCE NO.: 112:13143a, 13146a

TITLE: Hydrogenation of substituted
1-arylisouquinolin-3(2H)-ones to 5,6,7,8-tetrahydro-
and 1,4-dihydroisoquinolin-3(2H)-ones

AUTHOR(S): Hazai, Laszlo; Deak, Gyula; Toth, Gabor; Tamas, Jozsef
CORPORATE SOURCE: Inst. Exp. Med., Hung. Acad. Sci., Budapest, H-1450,
Hung.

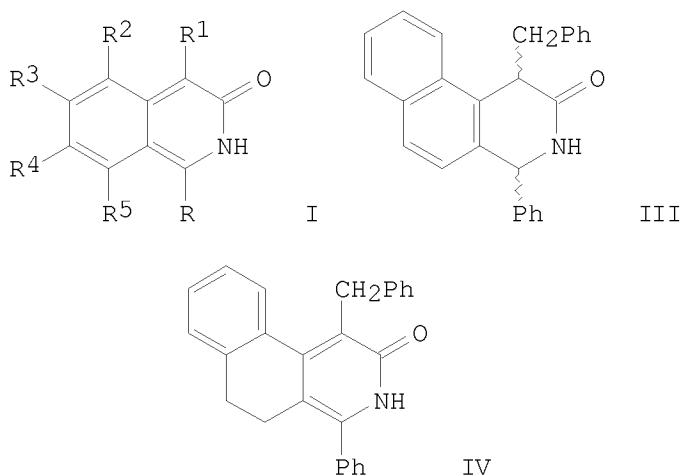
SOURCE: Journal of Heterocyclic Chemistry (1989),
26(3), 609-12

DOCUMENT TYPE: CODEN: JHTCAD; ISSN: 0022-152X

LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:76914

GI



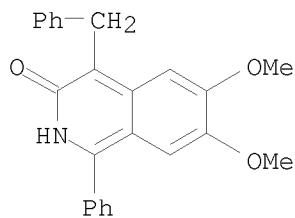
AB 1-Arylisoquinolin-3(2H)-ones I ($R = \text{Ph}$, 4-pyridyl, 4-pyridylmethyl; $R1 = H$, CH_2Ph , $\text{CH}_2\text{C}_6\text{H}_3(\text{OMe})_2$ -3,4; $R2 = H$, Me; $R3-R5 = H$; $R2R3$, $R4R5$ = benzo residue) were catalytically hydrogenated. Hydrogenation of I ($R = \text{Ph}$, $R1 = \text{CH}_2\text{Ph}$, $R2 = R3 = H$, $R4R5$ = benzo residue) (II) gave benz[f]isoquinolinone III as the main product and isomer IV as a byproduct.

IT 87748-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted catalytic hydrogenation of)

RN 87748-01-4 HCAPLUS

CN 3 (2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl-4-(phenylmethyl)- (CA INDEX
NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 110 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:35649 HCAPLUS

DOCUMENT NUMBER: 112:35649

ORIGINAL REFERENCE NO.: 112:6161a, 6164a

TITLE: Intramolecular reaction of 1-azaallylic anions and aryl halides: a synthesis of isoquinolines

AUTHOR(S): Kessar, Satinder V.; Singh, Paramjit; Dutt, Mahesh

CORPORATE SOURCE: Dep. Chem., Panjab Univ., Chandigarh, 160 014, India

SOURCE: Indian Journal of Chemistry, Section B: Organic

STN

Chemistry Including Medicinal Chemistry (1989)
), 28B(5), 365-6
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE:

LANGUAGE:

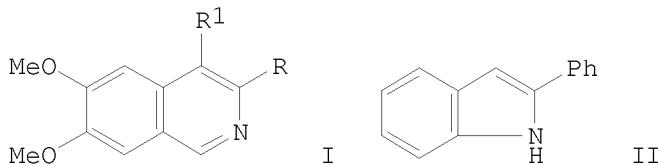
OTHER SOURCE(S):

GI

Journal

English

CASREACT 112:35649



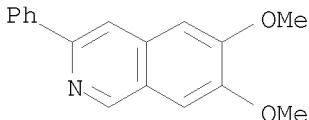
AB o-Halogenated N-benzylimines 2,4,5-Br(MeO)2C6H2CH2N:CRCH2R1 (R = Ph, SMe, R1 = H; R = H, R1 = Et) afford isoquinolines I on treatment with LiN(CHMe2)2 in THF (-78° to room temperature), while irradiation is needed for the cyclization of the corresponding N-phenylimine 2-ClC6H4N:CMePh to indole II.

IT 24285-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24285-10-7 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 111 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:614373 HCPLUS

DOCUMENT NUMBER: 111:214373

ORIGINAL REFERENCE NO.: 111:35553a, 35556a

TITLE: Synthesis and reactions of isoquinoline derivatives.

V. Synthesis and reactions of
3-chloroisooquinoline-4-carboxylic acids

Bartmann, Wilhelm; Konz, Elmar; Rueger, Wolfgang

Hoechst AG, Frankfurt/Main, D-6230, Fed. Rep. Ger.

Heterocycles (1989), 29(4), 707-18

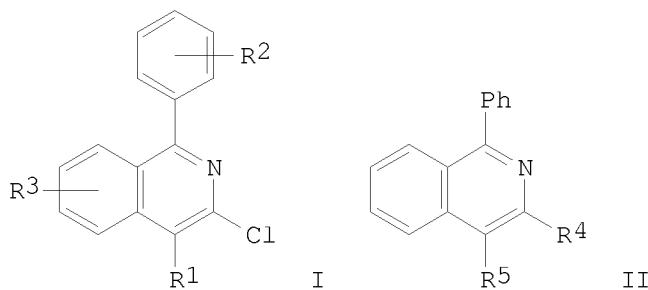
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:214373

GI



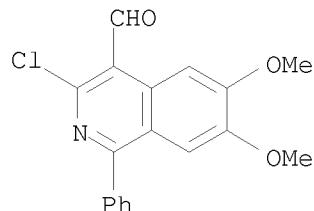
AB Aldehydes I ($R_1 = \text{CHO}$) ($R_2 = \text{H, Me, halo, NO}_2, \text{CF}_3$; $R_3 = \text{H, Me, halo, OMe}$) were oxidized by KMnO_4 to the resp. acids I ($R_1 = \text{CO}_2\text{H}$, $R_2 = R_3 = \text{H}$) was converted to isoquinolines II ($R_4 = \text{Cl, H, NH}_2$, substituted amino, alkoxy, OPh, SPh ; $R_5 = \text{CO}_2\text{H, CO}_2\text{Me, CONH}_2$, substituted carbamoyl, H).

IT 72179-16-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, by permanganate)

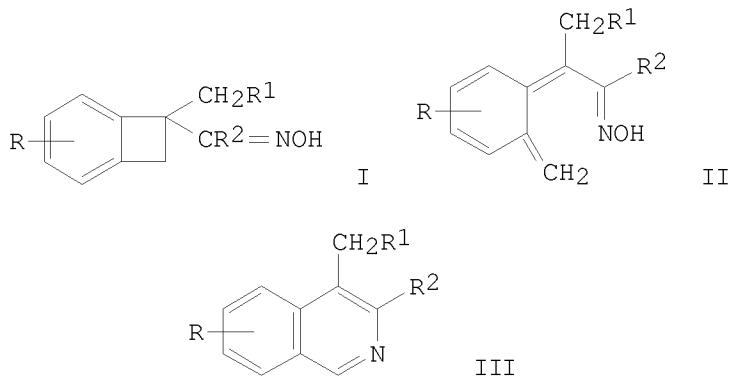
RN 72179-16-9 HCPLUS

CN 4-Isoquinolinecarboxaldehyde, 3-chloro-6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 112 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:594546 HCPLUS
DOCUMENT NUMBER: 111:194546
ORIGINAL REFERENCE NO.: 111:32335a, 32338a
TITLE: A convenient access to 3,4-disubstituted isoquinolines from benzocyclobut enyl ketoximes
AUTHOR(S): Shishido, Kozo; Hiroya, Kou; Fukumoto, Keiichiro;
Kametani, Tetsuji
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Heterocycles (1989), 28(1), 39-41
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:194546
GI



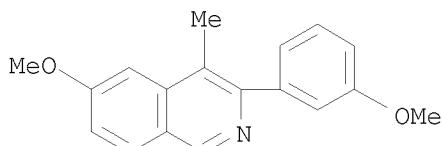
AB The thermolyses of several benzocyclobutenyl ketoximes I [R = 4-MeO, 5-MeO, R1 = H, R2 = Me; R = 5-MeO, R1 = H, R2 = Bu, cyclohexyl, 3,4-methylenedioxyphenyl, 3-MeOC₆H₄; R1 = Me, CH₂Ph, R2 = Me; R1R2 = (CH₂)₃] proceed via a preferential electrocyclic reaction of Z-*o*-quinonodimethane species II to yield 3,4-disubstituted isoquinolines III.

IT 122080-84-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 122080-84-6 HCPLUS

CN Isoquinoline, 6-methoxy-3-(3-methoxyphenyl)-4-methyl- (CA INDEX NAME)

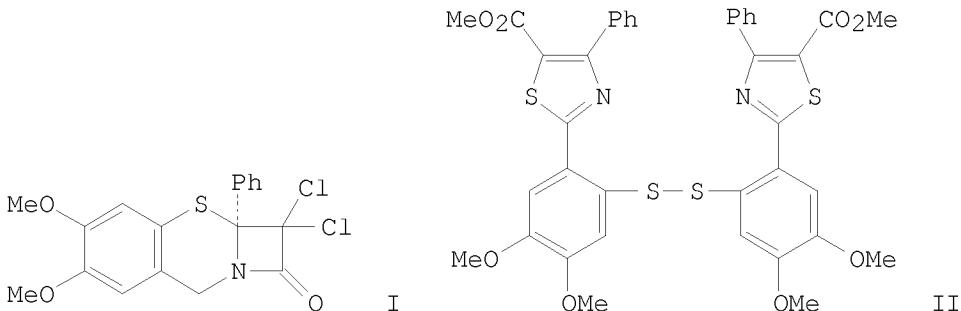


OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 113 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:533850 HCPLUS
DOCUMENT NUMBER: 111:133850
ORIGINAL REFERENCE NO.: 111:22395a, 22398a
TITLE: Ring transformations of 1,3-benzothiazine derivatives.
Part 4. Conversion of
6α-phenyl-7,7-dichloro-2,3-(2',3'-
dimethoxybenzo)-1-thiaoctem in the presence of base
AUTHOR(S): Fodor, Lajos; Szabo, Janos; Bernath, Gabor; Sohar,
Pal; Argay, Gyula; Kalman, Alajos; Tamas, Jozsef
CORPORATE SOURCE: Cent. Lab., Cty. Hosp., Gyula, H-5701, Hung.
SOURCE: Tetrahedron (1988), 44(23), 7181-4
DOCUMENT TYPE: Journal
LANGUAGE: English

STN

OTHER SOURCE(S): CASREACT 111:133850
GI



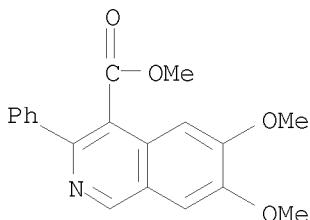
AB Treatment β -lactam I with base in MeOH led to a 1,4-benzothiazepine, a tetrasubstituted isoquinoline, and a thiazole disulfide derivative via a new ring transformation. The structure of the thiazole disulfide (II) was determined by x-ray diffraction.

IT 110694-90-1P

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in reaction of azetidinobenzothiazinone with base)

RN 110694-90-1 HCAPLUS

CN 4-Isoquinolinecarboxylic acid, 6,7-dimethoxy-3-phenyl-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 114 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:515004 HCAPLUS

DOCUMENT NUMBER: 111:115004

ORIGINAL REFERENCE NO.: 111:19283a, 19286a

TITLE: Reaction of 1,2-diarylethylamides with ethyl polyphosphate (EPP): correlation of the von Braun, Ritter and Bischler-Napieralski reactions

AUTHOR(S): Aguirre, J. M.; Alesso, E. N.; Ibanez, A. F.; Tombari, D. G.; Moltrasio Iglesias, G. Y.

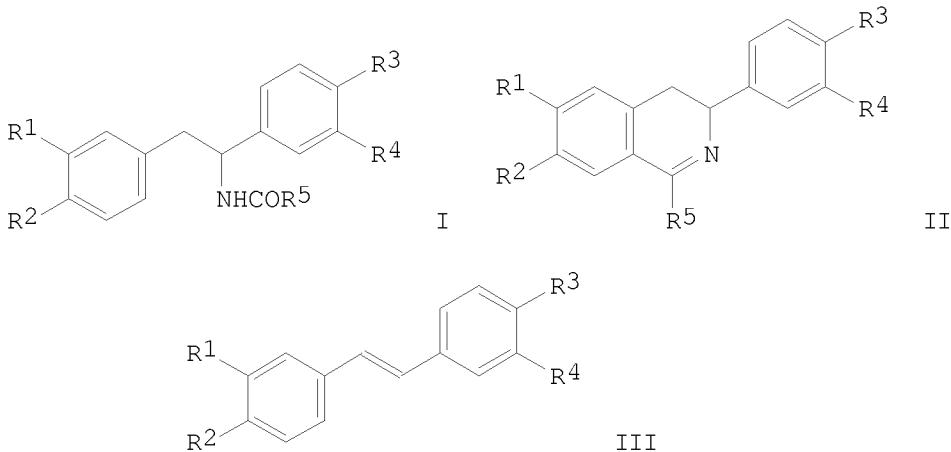
CORPORATE SOURCE: Dep. Bas. Sci., Natl. Univ. Lujan, Lujan, Argent.

SOURCE: Journal of Heterocyclic Chemistry (1989),
26(1), 25-7

CODEN: JHTCAD; ISSN: 0022-152X

STN

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:115004
GI

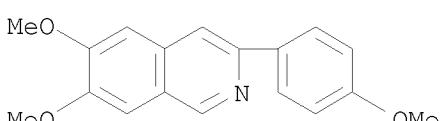


AB The Bischler-Napieralski cyclization of the 1,2-diarylethylamides I (R¹-R⁴ = H, OMe, R¹R² = OCH₂O, R¹ = H, R² = NO₂, R³ = R⁴ = OMe, R⁵ = H, Me) in a "one-pot" process using Et polyphosphate as the reagent only yields the dihydroisoquinolines II (R¹ = R² = OMe, R³ = R⁴ = H, R⁵ = H, Me; R¹ = OMe, R²-R⁵ = H; R¹ = R² = OMe, R³ = NO₂, R⁴ = R⁵ = H; R¹R² = OCH₂O, R³ = R⁴ = H, R⁵ = H, Me) in certain cases. The trans-stilbenes III and indans are obtained as neutral products and sometimes as sole products. Results clearly indicate the effect of aryl group substitution on the course of the reaction and the relationship between the Bischler-Napieralski and Ritter reactions.

IT 122200-66-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 122200-66-2 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-3-(4-methoxyphenyl)- (CA INDEX NAME)

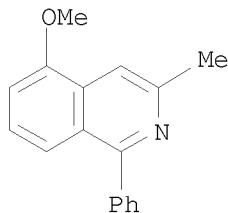


OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

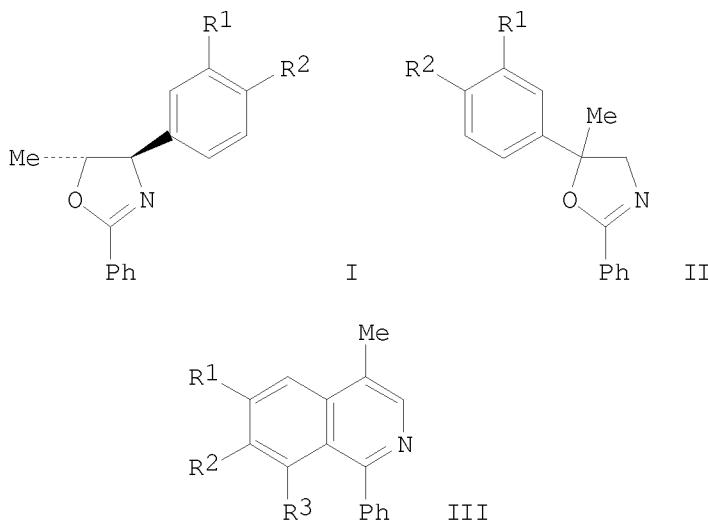
L13 ANSWER 115 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:422995 HCPLUS
DOCUMENT NUMBER: 111:22995
ORIGINAL REFERENCE NO.: 111:3989a,3992a
TITLE: Influence of substituents on basicity of isoquinolines

STN

AUTHOR(S): Zielinski, W.
CORPORATE SOURCE: Inst. Org. Chem. Technol., Silesian Polytech. Univ.,
Gliwice, Pol.
SOURCE: Studies in Organic Chemistry (Amsterdam) (1988
(Chem. Heterocycl. Compd.), 584-7
CODEN: SOCHDQ; ISSN: 0165-3253
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The pKa values for 1,3-dimethylisoquinoline, 1-phenyl-3-methylisoquinoline
and series of 5-, 6- and 7-substituted derivs. were determined in 50% aqueous
MeOH
by spectrophotometric method. The pKa values for 5-, 6-, and
7-substituted isoquinoline derivs. were correlated with Hammett σ
consts.
IT 78451-50-0
RL: PRP (Properties)
(basicity of)
RN 78451-50-0 HCPLUS
CN Isoquinoline, 5-methoxy-3-methyl-1-phenyl- (CA INDEX NAME)



L13 ANSWER 116 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:231483 HCPLUS
DOCUMENT NUMBER: 110:231483
ORIGINAL REFERENCE NO.: 110:38375a, 38378a
TITLE: Cyclization of 1-aryl-1-benzamidopropan-2-ols.
Formation of 4,5-dihydrooxazoles, rearranged
4,5-dihydrooxazoles, and isoquinolines
Fitton, Alan O.; Muzanila, Charles N.; Odusanya,
Olubunmi M.; Oppong-Boachie, Francis K.; Duckworth,
Stephen J.; Hadi, A. Hamid A.
AUTHOR(S): Dep. Chem. Appl. Chem., Univ. Salford, Salford, M5
4WT, UK
CORPORATE SOURCE: Journal of Chemical Research, Synopses (1988
(11), 352-3
SOURCE: CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:231483
GI



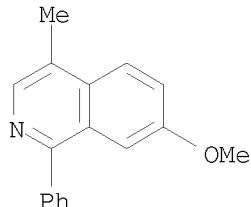
AB 1-Aryl-1-benzamido-2-propanols were treated with polyphosphoric acid to give 2-oxazolines I ($R_1 = H, OMe; R_2 = H, Me, OMe$) and rearrangement products II. I and isoquinolines III ($R_3 = H, OMe$) were obtained when P2O3 was used in xylene or decalin.

IT 120869-12-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 120869-12-7 HCPLUS

CN Isoquinoline, 7-methoxy-4-methyl-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 117 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:231407 HCPLUS

DOCUMENT NUMBER: 110:231407

ORIGINAL REFERENCE NO.: 110:38355a, 38358a

TITLE: A simple direct approach to 1-substituted

3-arylisouquinolines from deoxybenzoins and nitriles

Garcia, Alberto; Lete, Esther; Villa, M. Jesus;

Dominguez, Esther; Badia, M. Dolores

AUTHOR(S): Fac. Cienc., Univ. Pais Vasco, Bilbao, Spain

CORPORATE SOURCE: Tetrahedron (1988), 44(21), 6681-6

SOURCE: CODEN: TETRAB; ISSN: 0040-4020

STN

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:231407

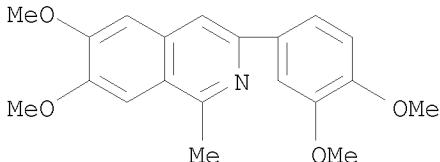
AB A new one-pot synthesis of 3-arylisouquinolines was accomplished by reaction of deoxybenzoins with an excess of nitriles and phosphorus pentoxide at room temperature. When the reaction was similarly carried out with phosphorus oxychloride instead of phosphorus pentoxide, the major product was a chlorostilbene derivative.

IT 35989-93-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35989-93-6 HCPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L13 ANSWER 118 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:212579 HCPLUS

DOCUMENT NUMBER: 110:212579

ORIGINAL REFERENCE NO.: 110:35275a, 35278a

TITLE: Hydroxyiminoisoquinolin-3(2H)-ones. VIII.

Acid-catalyzed ring contraction and Semmler-Wolff type rearrangement

AUTHOR(S): Tikk, Istvan; Deak, Gyula; Tamas, Jozsef

CORPORATE SOURCE: Inst. Exp. Med., Hung. Acad. Sci., Budapest, H-1450, Hung.

SOURCE: Acta Chimica Hungarica (1988), 125(2), 289-93

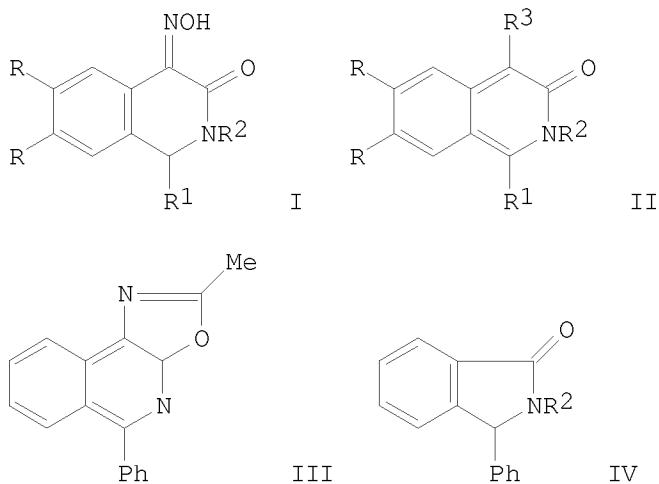
CODEN: ACHUDC; ISSN: 0231-3146

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:212579

GI

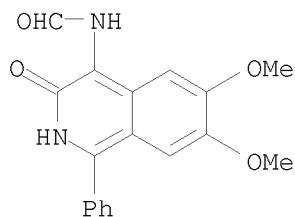


AB Refluxing isoquinolinone oximes I ($R = H, OMe, R1 = H, Ph, R2 = H, Me, Et$) in HCO_2H resulted in a rearrangement to give formamidoisoquinolinones II ($R, R1, R2, \text{ same}, R3 = NHCHO$). When $R1 = H$, the rearrangement was accompanied by deoximation and oxidation giving a multicomponent mixture. Acetylation of the deformylated II ($R = R2 = H, R1 = Ph, R3 = NH_2$) with Ac_2O in $AcOH$ gave either II ($R, R1, R2, \text{ same}, R3 = NHAc$) or oxazoloisoquinolinones III, depending on the reaction conditions. In polyphosphoric acid, I ($R = H, R1 = Ph, R2 = H, Me$) were converted by ring contraction to isoindolinones IV.

IT 120491-61-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 120491-61-4 HCPLUS

CN Formamide, N-(2,3-dihydro-6,7-dimethoxy-3-oxo-1-phenyl-4-isoquinolinyl)-
 (CA INDEX NAME)

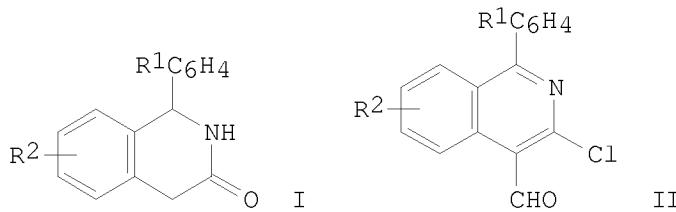


OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
 (3 CITINGS)

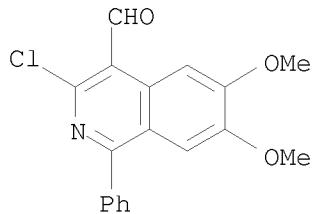
L13 ANSWER 119 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1989:192619 HCPLUS
 DOCUMENT NUMBER: 110:192619
 ORIGINAL REFERENCE NO.: 110:31969a,31972a
 TITLE: Synthesis and reactions of isoquinoline derivatives.
 II. Synthesis of

STN

AUTHOR(S): 3-chloroisoquinoline-4-carboxaldehydes
Bartmann, W.; Konz, E.; Rueger, W.
CORPORATE SOURCE: Hoechst A.-G., Frankfurt/Main, D-6230/80, Fed. Rep. Ger.
SOURCE: Synthesis (1988), (9), 680-3
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:192619
GI



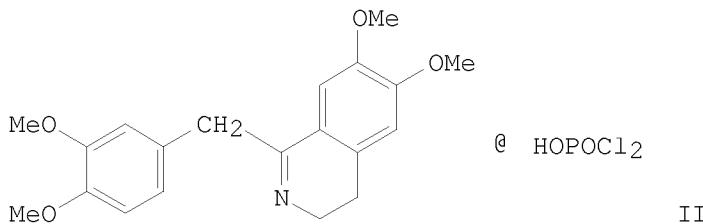
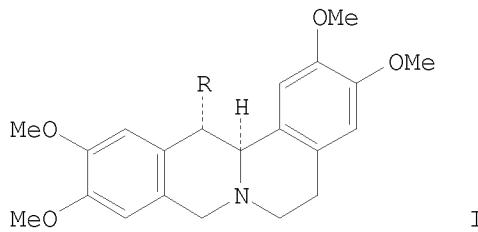
AB 1,4-Dihydro-3(2H)-isoquinolinones I [R1 = H, 2-Me, 2-F, 2,4-C12, R2 = H; R1 = H, R2 = 5-Me, 6-Me, 6-Cl, 6,7-(MeO)2, 6,7-Me2, etc.] are easily converted to 1-aryl-3-chloroisoquinoline-4-aldehydes II (same R's) via Vilsmeier-Haack reaction via an oxidation with KMnO4 under acidic conditions.
IT 72179-16-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 72179-16-9 HCPLUS
CN 4-Isoquinolinecarboxaldehyde, 3-chloro-6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 120 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:165652 HCPLUS
DOCUMENT NUMBER: 110:165652
ORIGINAL REFERENCE NO.: 110:27249a, 27252a
TITLE: 2,3,10,11-Tetramethoxy-5,6,7,8,13,13a - hexahydroprotoberberines and their B-seco analogs: synthesis and antineoplastic activity
AUTHOR(S): Sladkov, V. I.; Sazonova, N. M.; Grekova, G. S.; Kalistratov, S. G.; Sokolova, A. S.; Chernov, V. A.;

CORPORATE SOURCE: Suvorov, N. N.
 Mosk. Khim.-Tekhnol. Inst. im. Mendeleva, Moscow,
 USSR
 SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1989),
 23(1), 50-3
 CODEN: KHFZAN; ISSN: 0023-1134
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 110:165652
 GI



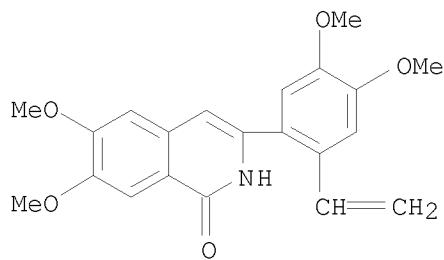
AB (\pm)-Xylopinine (I, R = H) and (\pm)-13 α -hydroxyxylopinine (I, R = OH) were prepared by the oxidation of II with O in alkaline medium followed by NaBH4 reduction and Pictet-Spengler cyclization of the resulting erythro-(\pm)- α -hydroxynorlaudanosine [for I (R = OH)] or by the NaBH4 reduction of II to (\pm)-norlaudanosine followed by Pictet-Spengler cyclization [for (\pm)-xylopinine]. Other derivs. of I were also synthesized. (\pm)-Xylopinine and its quaternary ammonium seco analog were toxic at ≥ 200 mg/kg in rats. All the compds. showed antitumor activity, with the most active being (\pm)-xylopinine. Seco analogs were less active.

IT 60315-12-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation and antitumor activity of)

RN 60315-12-0 HCPLUS

CN 1(2H)-Isoquinolinone, 3-(2-ethenyl-4,5-dimethoxyphenyl)-6,7-dimethoxy-
 (CA INDEX NAME)



L13 ANSWER 121 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:94964 HCPLUS

DOCUMENT NUMBER: 110:94964

ORIGINAL REFERENCE NO.: 110:15691a, 15694a

TITLE: Synthesis of 3-aryl-1-isoquinolines

AUTHOR(S): Villa, M. J.; Martinez de Marigorta, E.; Lete, E.; Dominguez, E.

CORPORATE SOURCE: Zientzi Fak., Euskal Herriko Unib., Bilbao, 48080, Spain

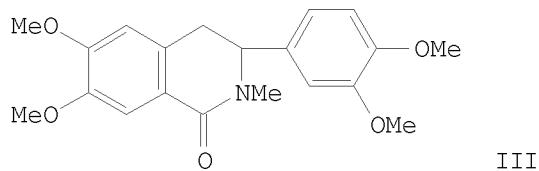
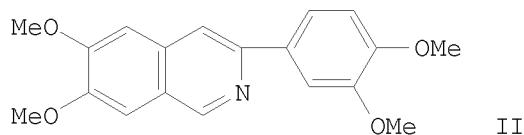
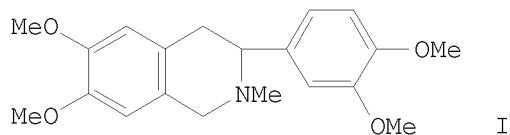
SOURCE: Elhuyar (1988), 14(1), 47-51

CODEN: ELHUDH; ISSN: 0212-1735

DOCUMENT TYPE: Journal

LANGUAGE: Basque

GI



AB MnO₂ or DDQ oxidation of the tetrahydroisoquinoline I and air oxidation of the corresponding dihydroisoquinoline methiodide all gave the isoquinoline II instead of the desired tetrahydroisoquinolinone III.

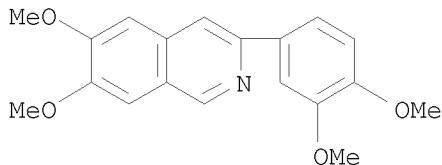
IT 69504-70-7P

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in oxidation of dihydro and tetrahydro derivs.)

RN 69504-70-7 HCPLUS

STN

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



L13 ANSWER 122 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:38849 HCPLUS

DOCUMENT NUMBER: 110:38849

ORIGINAL REFERENCE NO.: 110:6467a,6470a

TITLE: Direct synthesis of 3-alkyliisoquinolines with non-standard orientation of methoxy groups

Brovchenko, V. G.; Paidak, B. B.; Kuznetsov, E. V.

Nauchno-Issled. Inst. Fiz.-Org. Khim., Rostov. Gos. Univ., Rostov-on-Don, 344090, USSR

SOURCE: Khimiya Geterotsiklichesikh Soedinenii (1988), (1), 134-5

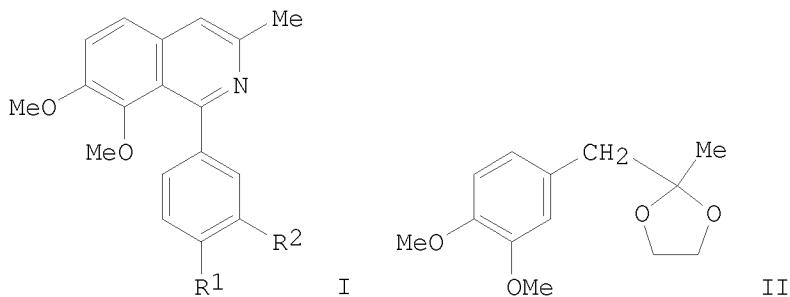
CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 110:38849

GI



AB Isoquinolines I ($R_1 = H, OMe$, $R_2 = H$; $R_1R_2 = OCH_2O$) were prepared from ketal II and the appropriate benzonitrile in 20-35% yield.

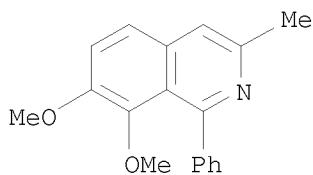
IT 118128-86-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

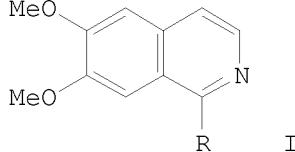
RN 118128-86-2 HCPLUS

CN Isoquinoline, 7,8-dimethoxy-3-methyl-1-phenyl- (CA INDEX NAME)

STN

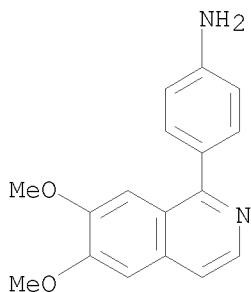


L13 ANSWER 123 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:583057 HCPLUS
DOCUMENT NUMBER: 109:183057
ORIGINAL REFERENCE NO.: 109:30129a,30132a
TITLE: A structure-activity relationship study on papaverine analogs
AUTHOR(S): Gupta, S. P.; Garg, Chhaya; Gupta, J. K.
CORPORATE SOURCE: Dep. Chem., Birla Inst. Technol. Sci., Pilani, 333031, India
SOURCE: Research Communications in Chemical Pathology and Pharmacology (1988), 61(2), 265-8
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



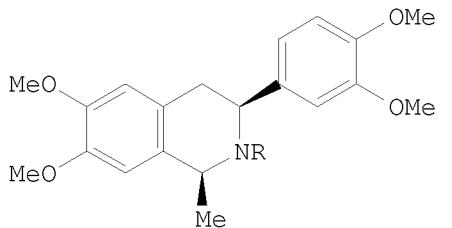
AB The structure-activity relations of papaverine analogs (I; R = p-substituted benzyl or Ph groups) as inhibitors of cAMP phosphodiesterase are discussed. The enzyme-inhibiting activity of these compds. is mainly controlled by hydrophobicity and steric factors. A significant quant. correlation was noted between the inhibitory activity and the van der Waals volume
IT 83633-12-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(cAMP phosphodiesterase inhibition by, structure in relation to)
RN 83633-12-9 HCPLUS
CN Benzenamine, 4-(6,7-dimethoxy-1-isoquinolinyl)- (CA INDEX NAME)

STN



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 124 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:570681 HCAPLUS
DOCUMENT NUMBER: 109:170681
ORIGINAL REFERENCE NO.: 109:28319a,28322a
TITLE: Reactivity of cis-1-methyl-3-aryltetrahydroisoquinoline towards N-alkylating agents
AUTHOR(S): Dominguez, E.; Badia, M. D.; Martinez de Marigorta, E.; Ezquerro, F.
CORPORATE SOURCE: Zientzi Fak., Euskal Herriko Unibertsitatea, Bilbao, Spain
SOURCE: Elhuyar (1987), 13(2), 78-84
DOCUMENT TYPE: CODEN: ELHUDH; ISSN: 0212-1735
LANGUAGE: Journal
GI Basque



I

AB N-Alkylation of the protoberberine intermediate I ($R = H$) gave low yields of I [$R = CH(OEt)_2$, 1,3-dioxolan-2-yl] together with I.HBr ($R = H$) and the aromatized isoquinoline, but no dibenzoquinolizinium product.

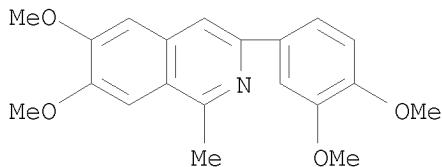
IT 35989-93-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35989-93-6 HCAPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)

STN



L13 ANSWER 125 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:493009 HCPLUS
DOCUMENT NUMBER: 109:93009
ORIGINAL REFERENCE NO.: 109:15525a,15528a
TITLE: Preparation of heterocyclic-substituted azoles as gastric secretion inhibitors and antiinflammatories
INVENTOR(S): Cox, David; Dowlatshahi, Hossein Ali; Hall, David Edward Hall; Ingall, Anthony Howard; Suschitzky, John Louis
PATENT ASSIGNEE(S): Fisons PLC, UK
SOURCE: Eur. Pat. Appl., 36 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 262845	A1	19880406	EP 1987-308318	19870921 <--
R: ES, GR				
WO 8802367	A1	19880407	WO 1987-GB656	19870921 <--
W: AU, DK, FI, JP, KR, NO				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8780244	A	19880421	AU 1987-80244	19870921 <--
AU 604771	B2	19910103		
EP 283504	A1	19880928	EP 1987-906433	19870921 <--
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 01501473	T	19890525	JP 1987-505851	19870921 <--
ZA 8707206	A	19880727	ZA 1987-7206	19870924 <--
US 4900751	A	19900213	US 1987-100584	19870924 <--
FI 8802394	A	19880520	FI 1988-2394	19880520 <--
DK 8802876	A	19880701	DK 1988-2876	19880525 <--
NO 8802321	A	19880711	NO 1988-2321	19880526 <--
PRIORITY APPLN. INFO.:				
		GB 1986-23299	A	19860927
		GB 1986-23301	A	19860927
		GB 1987-5017	A	19870304
		GB 1987-19644	A	19870820
		US 1986-918832	A2	19861014
		WO 1987-GB656	A	19870921

OTHER SOURCE(S): MARPAT 109:93009

GI For diagram(s), see printed CA Issue.

AB The title compds. [I; R1, R2 = H, alkyl; R1R2 = atoms to complete an (un)substituted, fused benzo or pyrido ring; R3-R10 = H, alkyl, PhCO, amino (un)modified CO2H, (un)substituted alkoxy, heterocyclyl, etc.; X = O, S, R12N; R12 = H, (un)substituted alkyl; A = 5- or 6-membered, fully unsatd. carbocycle or heterocycle; B = 5- or 6-membered, fully unsatd.,

STN

N-containing heterocycle; n = 0,1] and their pharmaceutically acceptable salts were prepared as gastric secretion and inflammation inhibitors (no data). 4-O2NC6H4N2+ BF4- was treated with 4-methoxypyridine 1-oxide to give 2-(4-methoxy-2-pyridinyl)-4-nitrophenol, which was esterified with Me2NCSCl and converted in 4 steps to give 4-(dimethylamino)-2-(4-methoxy-2-pyridinyl)phenyl disulfide. The latter was refluxed with 2-chlorobenzimidazole and NaBH3CN in HOAc/Me2CHOH to give (phenylthio)benzimidazole II.

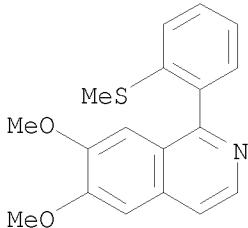
IT 115768-95-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of gastric secretion inhibitor)

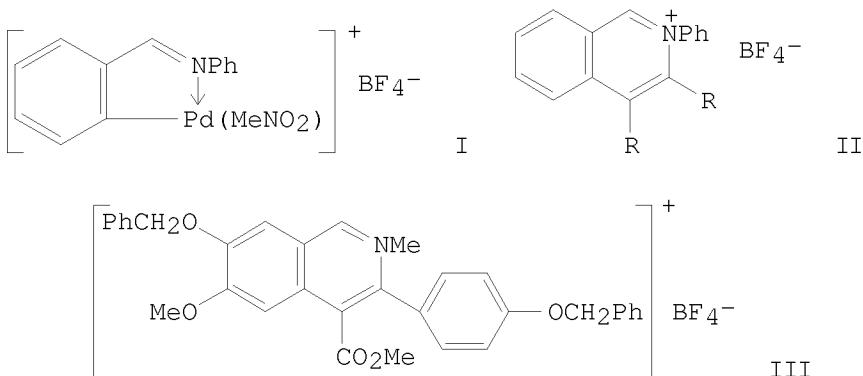
RN 115768-95-1 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-[2-(methylthio)phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 126 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:454944 HCPLUS
DOCUMENT NUMBER: 109:54944
ORIGINAL REFERENCE NO.: 109:9271a,9274a
TITLE: Isoquinolinium salt syntheses from cyclopalladated benzaldimines and alkynes
Wu, Guangzhong; Geib, Steven J.; Rheingold, Arnold L.; Heck, Richard F.
CORPORATE SOURCE: Cent. Catal. Sci. Technol., Univ. Delaware, Newark, DE, 19716, USA
SOURCE: Journal of Organic Chemistry (1988), 53(14), 3238-41
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:54944
GI



AB Cyclopalladated, N-substituted benzaldimine tetrafluoroborates react with disubstituted alkynes in poor to good yields to form isoquinolinium tetrafluoroborates. The reaction is particularly useful for preparing N,3,4-trisubstituted products. Electron-donating substituents may be present at the 5, 6, 7, and 8 positions, as well. Thus, cyclopalladated benzaldimine salt I, formed in situ from reaction of the cyclopalladated chloride dimer with AgBF₄ in MeNO₂, reacts with RC₂H₃ [R = Et, MeO₂C, (EtO)₂CH] to give isoquinolinium salts II (same R) in 12-80% yields. Me (p-benzoxyphenyl)propiolate adds to cyclopalladated N-methyl-3-benzoxy-4-methoxybenzaldimine tetrafluoroborate to form the 3-arylisquinolinium salt III. 3-Hexyne reacts with cyclopalladated N-phenylbenzaldimine chloro dimer at 150° to form the isoquinolinium chloride but at less than half (29%) the yield that is obtained from the corresponding tetrafluoroborate. The x-ray crystal structures of cyclopalladated N-methylbenzaldimine bis(dimethylformamide) tetrafluoroborate and III were determined.

IT 114943-90-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

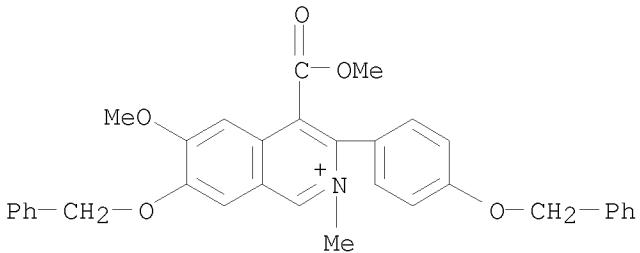
RN 114943-90-7 HCPLUS

CN Isoquinolinium, 6-methoxy-4-(methoxycarbonyl)-2-methyl-7-(phenylmethoxy)-3-[4-(phenylmethoxy)phenyl]-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

CRN 114943-89-4

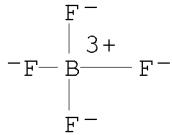
CMF C33 H30 N 05



STN

CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



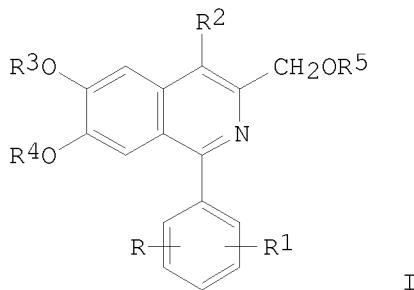
OS.CITING REF COUNT: 37 THERE ARE 37 CAPLUS RECORDS THAT CITE THIS RECORD (38 CITINGS)

L13 ANSWER 127 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:422849 HCAPLUS
DOCUMENT NUMBER: 109:22849
ORIGINAL REFERENCE NO.: 109:3904h,3905a
TITLE: Preparation of 3-(hydroxymethyl)isoquinolines as cardiotonics
INVENTOR(S): Rabloczky, Gyorgy; Korosi, Jeno; Lang, Tibor; Ling, Istvan; Hamori, Tamas; Kuhar, Maria; Elekes, Istvan; Botka, Peter; Varro, Andras; et al.
PATENT ASSIGNEE(S): EGIS Gyogyszergyar, Hung.
SOURCE: Brit. UK Pat. Appl., 17 pp.
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2190678	A	19871125	GB 1987-12047	19870521 <--
GB 2190678	B	19900620		
HU 44017	A2	19880128	HU 1986-2141	19860521 <--
HU 196758	B	19890130		
CH 673280	A5	19900228	CH 1987-1917	19870519 <--
US 4785104	A	19881115	US 1987-51767	19870520 <--
DK 8702582	A	19871122	DK 1987-2582	19870521 <--
FI 8702256	A	19871122	FI 1987-2256	19870521 <--
SE 8702119	A	19871122	SE 1987-2119	19870521 <--
FR 2599033	A1	19871127	FR 1987-7119	19870521 <--
NL 8701214	A	19871216	NL 1987-1214	19870521 <--
DE 3717079	A1	19880107	DE 1987-3717079	19870521 <--
JP 63039863	A	19880220	JP 1987-124993	19870521 <--
ES 2005583	A6	19890316	ES 1987-1497	19870521 <--
BE 1000719	A4	19890321	BE 1987-572	19870521 <--
CS 264293	B2	19890613	CS 1987-3691	19870521 <--
DD 268940	A5	19890614	DD 1987-303003	19870521 <--
SU 1551245	A3	19900315	SU 1987-4202630	19870521 <--
PRIORITY APPLN. INFO.:			HU 1986-2141	A 19860521

STN

OTHER SOURCE(S): MARPAT 109:22849
GI

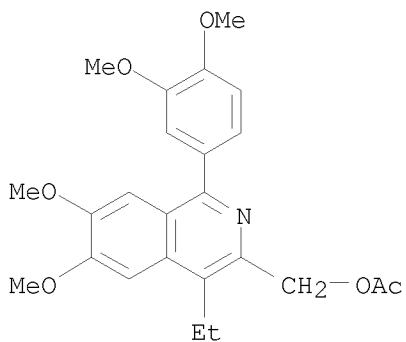


AB The title compds. I ($R, R_1 = H, \text{halo}, \text{NO}_2, \text{C1-4 alkoxy}$; $R_2, R_3, R_4 = \text{C1-4 alkyl}$; $R_3R_4 = \text{CH}_2$; $R_5 = \text{H}$) were prepared by hydrolysis of I ($R_5 = \text{acyl}$). 1-(3,4-Dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisoquinoline N-oxide was refluxed with Ac_2O 2.5 h to give 84.1% I ($R = 3\text{-MeO}$, $R_1 = 4\text{-MeO}$, $R_2 = \text{Et}$, $R_3 = R_4 = \text{Me}$, $R_5 = \text{Ac}$). Similarly prepared I ($R = 3\text{-Cl}$, $R_1 = R_2 = \text{H}$, $R_3 = R_4 = \text{Me}$, $R_5 = \text{Ac}$) was refluxed in 5% aqueous HCl to give 82.4% I. HCl ($R = 3\text{-Cl}$, $R_1 = R_2 = R_5 = \text{H}$, $R_3 = R_4 = \text{Me}$) (II) which, at 5 mg/kg i.v., gave a 50% increase in myocardial contractile force in anesthetized open-chest cats. Tablets were prepared containing II 10, lactose 185, cellulose 25, talc 5, starch 73, and Mg stearate 2 g per 103.

IT 114920-02-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of cardiotonics)

RN 114920-02-4 HCPLUS

CN 3-Isoquinolinemethanol, 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-, 3-acetate (CA INDEX NAME)



L13 ANSWER 128 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:228395 HCPLUS
DOCUMENT NUMBER: 108:228395

STN

ORIGINAL REFERENCE NO.: 108:37365a, 37368a
TITLE: Electrochemical reduction of a 5H-2,3-benzodiazepine
AUTHOR(S): Fuhlendorff, Rene; Lund, Henning
CORPORATE SOURCE: Dep. Chem., Univ. Aarhus, Arhus, DK-8000, Den.
SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1988), B42(1), 52-4
CODEN: ACBOCV; ISSN: 0302-4369

DOCUMENT TYPE: Journal
LANGUAGE: English

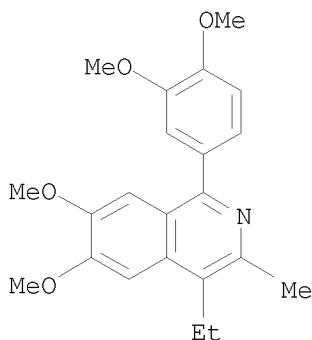
AB Exptl. work was carried out on 2 compds.: 7,8-dimethoxy-1-(3,4-dimethoxyphenyl)-5-ethyl-4-methyl-5H-2,3-benzodiazepine (Tofisopam) (I) and on the model compound benzophenone cyclohexanone azine (II). The polarog. of II in 40% aqueous DMF at pH 1 gave two 2-electron waves at E_{1/2} = -0.55 and -0.70 V (vs. SCE). Several conditions were imposed, and the various results and mechanisms are discussed. For compound I, the redns. were carried out in 0.2M HCl containing 0.5M KCl and also in DMF/0.10M Bu₄NI containing an excess of PhOH at -1.85 V (vs. Ag/AgI). In the latter reduction, 2 diastereomeric 1,2-dihydro-7,8-dimethoxy-1-(3,4-dimethoxyphenyl)-5-ethyl-4-methyl-5H-2,3-benzodiazepines were formed.

IT 1616-49-5P

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by electrochem. reduction)

RN 1616-49-5 HCPLUS

CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

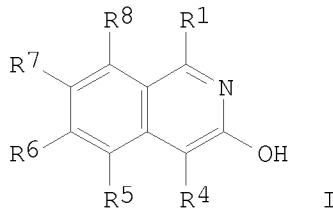
L13 ANSWER 129 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:186593 HCPLUS
DOCUMENT NUMBER: 108:186593
ORIGINAL REFERENCE NO.: 108:30654h, 30655a
TITLE: Preparation and formulation of 4-N-substituted isoquinolinol compounds having cardiotonic, phosphodiesterase fraction III inhibiting properties, and/or renal vasodilating properties
INVENTOR(S): Kanojia, Ramesh M.; Falotico, Robert; Tobia, Alfonso J.; Press, Jeffery B.

STN

PATENT ASSIGNEE(S): Ortho Pharmaceutical Corp., USA
SOURCE: U.S., 11 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4714705	A	19871222	US 1986-882655	19860707 <--
DK 8703480	A	19880108	DK 1987-3480	19870706 <--
FI 8702980	A	19880108	FI 1987-2980	19870706 <--
NO 8702812	A	19880108	NO 1987-2812	19870706 <--
AU 8775273	A	19880114	AU 1987-75273	19870706 <--
AU 597083	B2	19900524		
ZA 8704894	A	19890222	ZA 1987-4894	19870706 <--
IL 83088	A	19910816	IL 1987-83088	19870706 <--
EP 252721	A1	19880113	EP 1987-306002	19870707 <--
EP 252721	B1	19911002		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 63022562	A	19880130	JP 1987-167955	19870707 <--
CN 87105724	A	19880309	CN 1987-105724	19870707 <--
HU 44515	A2	19880328	HU 1987-3058	19870707 <--
HU 196966	B	19890228		
AT 67992	T	19911015	AT 1987-306002	19870707 <--
ES 2040750	T3	19931101	ES 1987-306002	19870707 <--
PRIORITY APPLN. INFO.:			US 1986-882655	A 19860707
			EP 1987-306002	A 19870707

OTHER SOURCE(S): CASREACT 108:186593
GI



AB The title compds. I [R1 = H, (halo)alkyl, (halo)Ph, (halo)naphthyl; R4 = NO₂, NO, NH₂, di-C₁-5-alkylamino, NHCO(Y)(R)n; R = H, alkyl, C₃-6 cycloalkyl, Ph, naphthyl, etc.; Y = O, N(H)x; R₅, R₆, R₇, R₈ = H, halo, HO, alkoxy; R₅R₆, R₆R₇, R₇R₈ = OCH₂O; x, n = 0-2] and their pharmaceutical salts, were prepared I (R1 = Me; R4 = NH₂; R6, R7 = MeO) as the diacetate solvate in AcOH at room temperature was reacted with Me(CH₂)₂CH₂NCO to give I (R1 = Me; R4 = BuNHCONH; R6, R7 = MeO) (III). III and other I each exhibited 1 or more of cardiotonic and renal vasodilating properties and phosphodiesterase fraction III inhibiting properties.

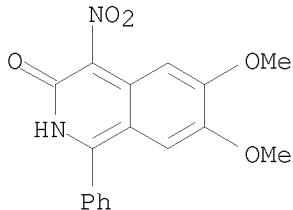
IT 113982-83-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

STN

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as drug)

RN 113982-83-5 HCAPLUS

CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-4-nitro-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 130 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1988:186498 HCAPLUS

DOCUMENT NUMBER: 108:186498

ORIGINAL REFERENCE NO.: 108:30635a,30638a

TITLE: Benzopyrylium salts. 30. Synthesis and properties of
2-benzopyrylium salts with 2,6-di-tert-butylphenol
group in position 3

AUTHOR(S): Shcherbakova, I. V.; Ukhin, L. Yu.; Komissarov, V. N.;
Kuznetsov, E. V.; Polyakov, A. V.; Yanovskii, A. I.;
Struchkov, Yu. T.

CORPORATE SOURCE: Inst. Fiz. Org. Khim., Rostov, USSR

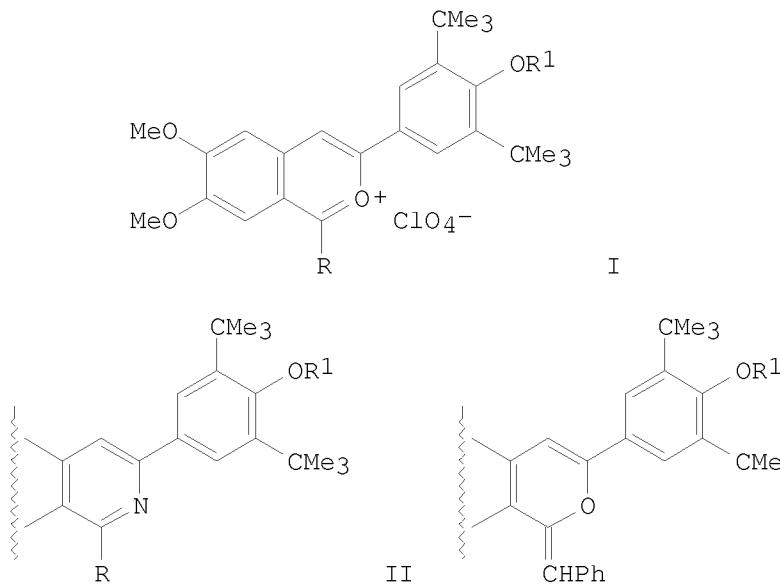
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1987
(8), 1032-8

DOCUMENT TYPE: CODEN: KGSSAQ; ISSN: 0453-8234

LANGUAGE: Journal

OTHER SOURCE(S): Russian

GI

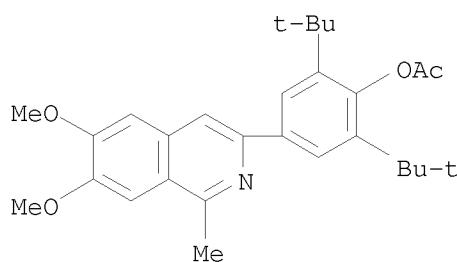


AB 2-Benzopyrylium perchlorates I ($R = Me, Ph, R1 = Ac; R = PhCH_2, Ph, R1 = H; R = PhCH_2, R1 = COCH_2Ph$), prepared by acylation of 3,5-di-tert-butyl-4-hydroxy-3',4'-dimethoxybenzoin in the presence of 70% $HClO_4$, were treated with NH_4OAc in $AcOH$ to give isoquinolines II ($R = Me, R1 = Ac; R = PhCH_2, R1 = H$). Addnl. obtained were benzopyran derivs. III ($R1 = H, COCH_2Ph$).

IT 114261-70-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

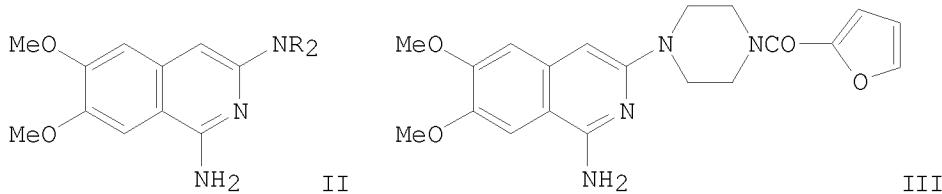
RN 114261-70-0 HCPLUS

CN Phenol, 4-(6,7-dimethoxy-1-methyl-3-isoquinolinyl)-2,6-bis(1,1-dimethylethyl)-, 1-acetate (CA INDEX NAME)



L13 ANSWER 131 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1988:167273 HCPLUS
 DOCUMENT NUMBER: 108:167273
 ORIGINAL REFERENCE NO.: 108:27493a
 TITLE: 1,3-Diamino-6,7-dimethoxyisoquinoline derivatives as potential α_1 -adrenoceptor antagonists
 AUTHOR(S): Bordner, Jon; Campbell, Simon F.; Palmer, Michael J.;

CORPORATE SOURCE: Tute, Michael S.
SOURCE: Dep. Discovery Chem., Pfizer Cent. Res.,
Sandwich/Kent, UK
DOCUMENT TYPE: Journal of Medicinal Chemistry (1988),
31(5), 1036-9
LANGUAGE: CODEN: JMCMAR; ISSN: 0022-2623
OTHER SOURCE(S): Journal
GI English
CASREACT 108:167273



AB Treatment of 2,4,5-Me(MeO)2C6H2CN (**I**) with LiN(CHMe₂)₂ followed by reaction with R2NCN [R = Me, R2 = (CH₂)₅] provided 1,3-diamino-6,7-dimethoxyisoquinolines **II** (R = as above), which were evaluated for α -adrenoceptor binding affinity and antihypertensive activity. **II** (R = Me) showed no significant affinity for α 1-adrenoceptors, while the 3-(2-furoyl-1-piperazinyl) analog **III**, prepared from **I** and 1-cyano-4-(tert-butoxycarbonyl)piperazine in 3 steps, was 1000-fold less potent than prazosin. PKa data showed that 34% N(2) protonation of **II** (R = Me) (pKa = 7.1) would occur at physiol. pH, in agreement with x-ray crystallog. anal. of **III.HCl**. Comparison of pos. charge distribution following protonation of **II** (R = Me) with the corresponding quinoline and quinazoline cations confirmed that N(1) protonation is required for these heterocyclic nuclei to bind efficiently to the α 1-adrenoceptor. Computer-assisted comparison of the x-ray structures of **III.HCl** and prazosin suggested that the 4.0 kcal/mol difference in α 1-adrenoceptor binding energies was largely due to salt-bridge formation (ca. 3.0 kcal/mol) between the protonated quinazoline and the receptor protein. Neither **II** nor **III** were effective antihypertensive agents in rats even when administered at relatively high doses (10 mg/kg). These results support the hypothesis that the antihypertensive activity of prazosin, doxazosin, and related compds. derives solely from α 1-adrenoceptor blocking.

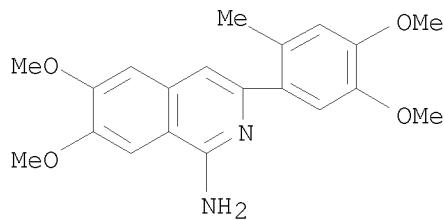
IT 23023-37-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and protonation of, with hydrogen chloride)

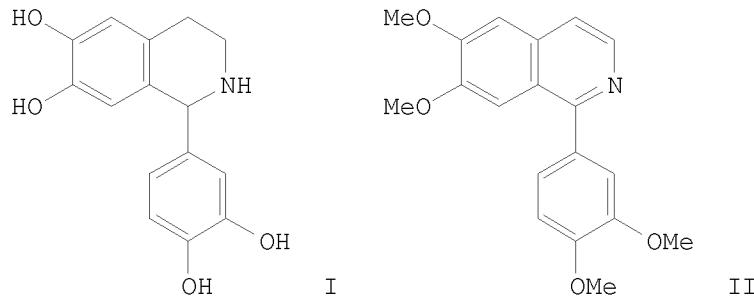
RN 23023-37-2 HCAPLUS

CN 1-Isoquinolinamine, 3-(4,5-dimethoxy-2-methylphenyl)-6,7-dimethoxy- (CA INDEX NAME)

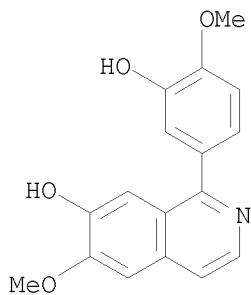


OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(10 CITINGS)

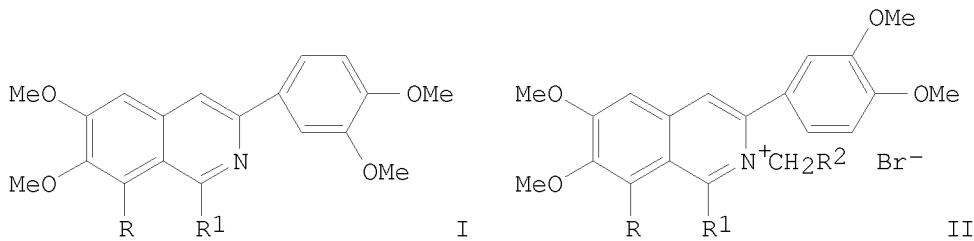
L13 ANSWER 132 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:131545 HCPLUS
DOCUMENT NUMBER: 108:131545
ORIGINAL REFERENCE NO.: 108:21571a, 21574a
TITLE: Novel (\pm)-1-phenyltetrahydroisoquinolines and 1-phenylisoquinolines: potential intermediates in alkaloid synthesis
AUTHOR(S): Venugopalan, Bindumadhavan; Brossi, Arnold
CORPORATE SOURCE: Lab. Chem., Natl. Arthritis Inst., Bethesda, MD, 20892, USA
SOURCE: Heterocycles (1987), 25(1), 259-64
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:131545
GI



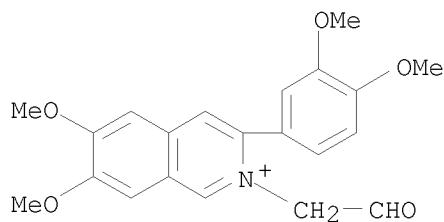
AB The synthesis of several novel (\pm)-1-phenyltetrahydroisoquinolines, e.g., I, and 1-phenylisoquinolines, e.g. II, structurally related to the 1-benzylisoquinoline alkaloids norreticuline, reticuline, tetrahydropapaveroline and papaverine, by the Bischler-Napieralski route is reported.
IT 113332-69-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-methylation of)
RN 113332-69-7 HCPLUS
CN 7-Isoquinolinol, 1-(3-hydroxy-4-methoxyphenyl)-6-methoxy- (CA INDEX NAME)



L13 ANSWER 133 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1988:112176 HCPLUS
 DOCUMENT NUMBER: 108:112176
 ORIGINAL REFERENCE NO.: 108:18365a,18368a
 TITLE: N-Alkylation of 3-arylisoquinoline derivatives
 AUTHOR(S): Badia, M. D.; Dominguez, E.; Izagirre, J. K.; Martinez de Marigorta, E.
 CORPORATE SOURCE: Kim. Org. Lab., Zientzi Fak., Bilbao, Spain
 SOURCE: Elhuyar (1987), 13(1), 39-41
 CODEN: ELHUDH; ISSN: 0212-1735
 DOCUMENT TYPE: Journal
 LANGUAGE: Basque
 GI



AB Alkylation of isoquinolines I ($R = R_1 = H$; $R = H, OMe$, $R_1 = Me$) with $BrCH_2R_2$ [$R_2 = CHO, CH(OH)_2$] in a variety of solvents and conditions gave only the quaternized derivs. II.
 IT 23158-18-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 23158-18-1 HCPLUS
 CN Isoquinolinium, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-2-(2-oxoethyl)-, bromide (1:1) (CA INDEX NAME)



L13 ANSWER 134 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1988:37612 HCPLUS

DOCUMENT NUMBER: 108:37612

ORIGINAL REFERENCE NO.: 108:6287a,6290a

TITLE: (Hydroxyimino)isoquinolin-3(2H)-ones. Part 7.

Rearrangement of

4-(hydroxyimino)-1,4-dihydroisoquinolin-3(2H)-ones under Wolff-Semmler type reaction conditions

AUTHOR(S): Tikk, Istvan; Deak, Gyula; Sohar, Pal; Tamas, Jozsef
CORPORATE SOURCE: Inst. Exp. Med., Budapest, H-1083, Hung.

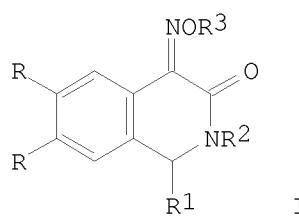
SOURCE: Journal of Chemical Research, Synopses (1987), (4), 95

DOCUMENT TYPE: CODEN: JRPSDC; ISSN: 0308-2342

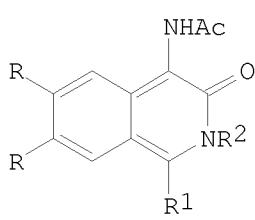
LANGUAGE: Journal

OTHER SOURCE(S): English

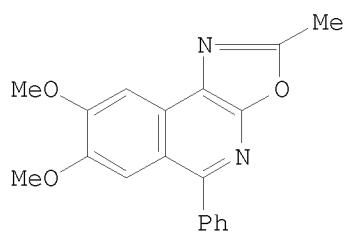
GI: CASREACT 108:37612



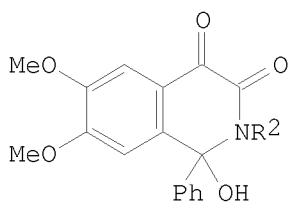
I



II



III



IV

AB Rearrangement of the title oximes I (R = H, MeO; R1 = Ph, 4-ClC₆H₄; R2 = H, Me; R3 = H) in refluxing AcOH-Ac₂O containing HCl (Beckmann's mixture) gave

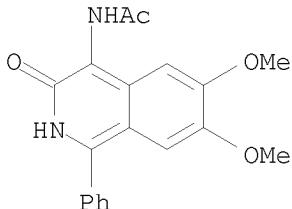
(acylamino)isoquinolinones II. Treatment of I ($R = R_2 = R_3 = H$; $R_1 = Ph$) with Beckmann's mixture at 50° gave I ($R = R_2 = H$, $R_1 = Ph$, $R_3 = Ac$). Treatment of methoxy derivative I ($R = MeO$; $R_1 = Ph$; $R_2 = R_3 = H$) with Ac₂O at 50° gave monoacyl derivative I ($R_2 = Ac$, $R_3 = H$) and at 135° gave diacyl derivative I ($R_2 = R_3 = Ac$), while treatment with Beckmann's mixture

at 95° gave oxazoloisoquinoline III. Treatment of I ($R = MeO$; $R_1 = Ph$; $R_2 = H$, Me ; $R_3 = H$) with Beckmann's mixture at 55° gave deoximated and oxidized derivs. IV ($R_2 = H$, Me). Reduction of IV with NaBH₄ gave 4,5,2-(MeO)₂(HOCHPh)C₆H₂CH(OH)CONHR₂ (V; $R_2 = H$, Me). V ($R_2 = H$) is a single diastereomer, while V ($R_2 = Me$) is a mixture of diastereomers.

IT 112010-86-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 112010-86-3 HCPLUS

CN Acetamide, N-(2,3-dihydro-6,7-dimethoxy-3-oxo-1-phenyl-4-isooquinolinyl)-
(CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 135 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1988:33983 HCPLUS

DOCUMENT NUMBER: 108:33983

ORIGINAL REFERENCE NO.: 108:5629a,5632a

TITLE: Inhibition of NADH oxidase and lactate dehydrogenase of *Mycoplasma gallisepticum* by copper complexes of 2,2'-bipyridyl analogs

AUTHOR(S): Gaisser, H. Dieter; De Vries, John; Van der Goot, Henk; Timmerman, Henk

CORPORATE SOURCE: Dep. Pharmacochem., Vrije Univ., Amsterdam, 1081 HV, Neth.

SOURCE: Biochemical Pharmacology (1987), 36(19), 3237-41

CODEN: BCPCA6; ISSN: 0006-2952

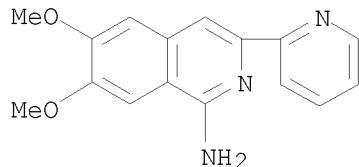
DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the presence of Cu²⁺, 2,2'-bipyridyl analogs possess growth-inhibitory activity against *M. gallisepticum*. The inhibition of the energy-yielding metabolism plays a role in the mechanism of action. Apparently, the inhibition of lactate dehydrogenase and NADH oxidase was involved. Both enzymes were inhibited *in vitro* and *in vivo* by several Cu-2,2'-bipyridyl complexes. A 2-step mechanism of action was proposed; first a Cu complex enters the cell; then, after dissociation of the complex, the enzymes are inhibited by free Cu²⁺.

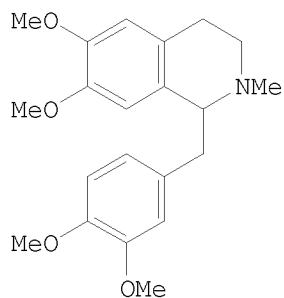
STN

IT 69767-44-8D, copper complexes
RL: BIOL (Biological study)
(lactate dehydrogenase and NADH oxidase of *Mycoplasma gallisepticum*
inhibition by, kinetics of)
RN 69767-44-8 HCPLUS
CN 1-Isoquinolinamine, 6,7-dimethoxy-3-(2-pyridinyl)- (CA INDEX NAME)

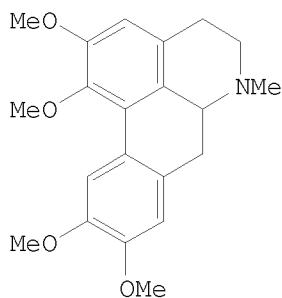


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 136 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1987:637093 HCPLUS
DOCUMENT NUMBER: 107:237093
ORIGINAL REFERENCE NO.: 107:38104h,38105a
TITLE: Ruthenium(IV) tetrakis(trifluoroacetate), a new
oxidizing agent. III. An efficient access to the
aporphine and homoaporphine skeletons and their
structural studies
AUTHOR(S): Landais, Y.; Rambault, D.; Robin, J. P.
CORPORATE SOURCE: Fac. Sci., Univ. Maine, Le Mans, 72017, Fr.
SOURCE: Tetrahedron Letters (1987), 28(5), 543-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:237093
GI



I



II

AB The title reagent (RUTFA) couples efficiently
phenylalkyltetrahydroisoquinolines, e.g. I, and the syntheses of glaucine
(II), thalicsimidine and homoglaucine were carried out. The
stereostructures of the aporphine and homoaporphine skeletons were determined
by using PMR at 500 MHz.
IT 111427-25-9P

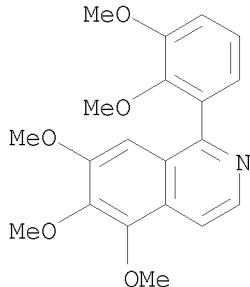
STN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and attempted intramol. cyclization of)

RN 111427-25-9 HCPLUS

CN Isoquinoline, 1-(2,3-dimethoxyphenyl)-5,6,7-trimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS
RECORD (14 CITINGS)

L13 ANSWER 137 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1987:617500 HCPLUS

DOCUMENT NUMBER: 107:217500

ORIGINAL REFERENCE NO.: 107:34891a,34894a

TITLE: New isoquinoline derivatives, procedure for their
preparation, pharmaceutical preparations containing
them, and their use as psychotropics

INVENTOR(S): Konz, Elmar; Rueger, Wolfgang; Kruse, Hansjoerg

PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.

SOURCE: Ger. Offen., 14 pp.

CODEN: GWXXBX

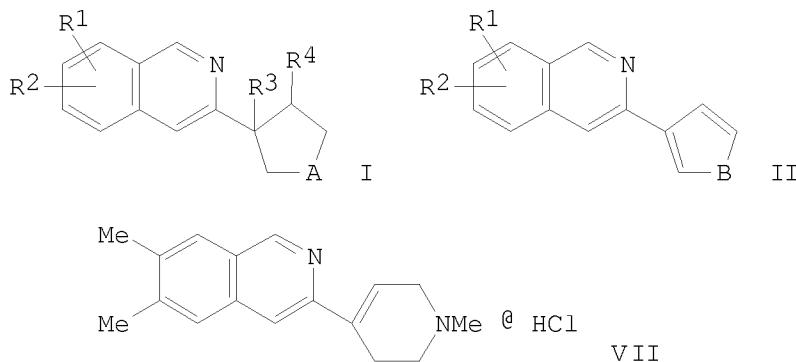
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3604754	A1	19870820	DE 1986-3604754	19860214 <--
PRIORITY APPLN. INFO.:			DE 1986-3604754	19860214
OTHER SOURCE(S):	CASREACT	107:217500		
GI				



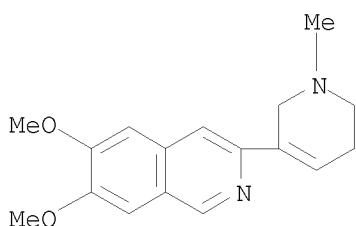
AB Isoquinolines I [R1, R2 = H, halo, OH, NO₂, NH₂, C1-6 alkyl, alkoxy, PhCH₂O, OCH₂O, OCH₂CH₂O; R3, R4 = H, R₃R₄ = bond; A = NR₅CH₂, CH₂NR₅, R₅ = H, PhCH₂, C1-6 alkyl or C2-6 alkenyl, each (un)substituted with Bz or 4-halobenzoyl] and their physiol. tolerable salts with acids, useful as psychotropics showing inhibition of tetrabenazine-induced ptosis in mice and of resumption of serotonin in synaptosomes and potentiation of 5-hydroxytryptophan-induced head twitching of mice, were prepared Reaction of isoquinoline II (R1, R2 as above, B = N:CH, CH:N) with alkylating agent ZR5' [Z = leaving group, R5' = PhCH₂, C1-6 alkyl or C2-6 alkenyl (un)substituted with Bz or 4-halobenzoyl (CO may be in protected form)] and reduction of the obtained quaternary pyridinium salt with a complex metal hydride to give I (R1, R2 as above, R₃R₄ = bond, R₅ = R5') and optional cleavage of any protection and the obtained I optionally a) when R5 = PhCH₂, debenzylated to R5 = H; or b) where R₃R₄ = bond, catalytically hydrogenated to I (R3 = R4 = H); or c) where R1 and/or R2 = alkoxy, PhCH₂O, OCH₂O, or OCH₂CH₂O, converted into I (R1 and/or R2 = OH; or d) alkylating I (R5 = H) to I [R5 = PhCH₂, C1-6 alkyl or C2-6 alkenyl (un)substituted with Bz or 4-halobenzyl] gave I. Et isonicotinate, 3,4-Me₂C₆H₃CH₂CN, and ethanolic NaOEt reacted to give α-cyano-3,4-dimethylbenzyl 4-pyridyl ketone, hydrolysis of which gave 3,4-dimethylbenzyl 4-pyridyl ketone (III) which was converted via (3,4-dimethyl-2-phenyl)-1-(4-pyridyl)ethylamine (IV) and 98% N-[2-(3,4-dimethylphenyl)-1-(4-pyridyl)ethyl]formamide (V) to 6,7-dimethyl-3-(4-pyridyl)isoquinoline (VI) and some of the 7,8-di-Me isomer. Quaternization with MeI and treatment of the pyridinium salt with aqueous NaOH and NaBH₄ gave tetrahydropiperidine VII. The ED₅₀ of VII against tetrabenazine-induced ptosis in mice was 9.9 mg/kg orally.

IT 111332-72-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(partial ether cleavage of)

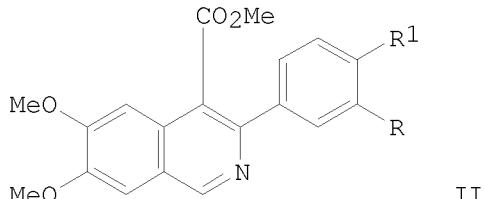
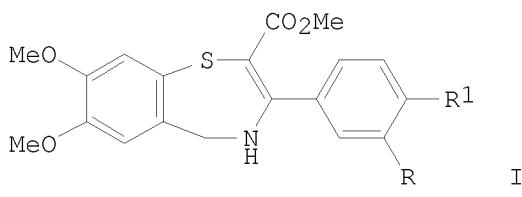
RN 111332-72-0 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-3-(1,2,5,6-tetrahydro-1-methyl-3-pyridinyl)- (CA INDEX NAME)

STN



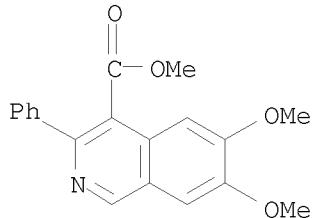
L13 ANSWER 138 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1987:575851 HCPLUS
DOCUMENT NUMBER: 107:175851
ORIGINAL REFERENCE NO.: 107:28223a, 28226a
TITLE: Sulfur extrusion from 1,4-benzothiazepines. Formation of 3-aryl-4-carbomethoxyisoquinolines
AUTHOR(S): Fodor, Lajos; MacLean, David B.
CORPORATE SOURCE: Dep. Chem., McMaster Univ., Hamilton, ON, L8S 4M1, Can.
SOURCE: Canadian Journal of Chemistry (1987), 65(1), 18-20
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:175851
GI



AB Treatment of benzothiazepines I ($R = R1 = H$, OMe ; $RR1 = OCH2O$) with N -chlorosuccinimide in ether gave isoquinolines II (yields 68.7, 56.4, and 61%, resp.) in a reaction in which the sulfur atom was extruded from the seven-membered thiazepin ring.
IT 110694-90-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 110694-90-1 HCPLUS
CN 4-Isoquinolinecarboxylic acid, 6,7-dimethoxy-3-phenyl-, methyl ester (CA

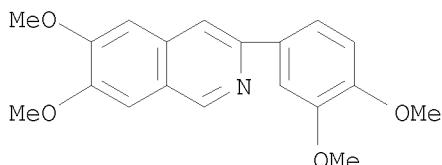
STN

INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

L13 ANSWER 139 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1987:403691 HCAPLUS
DOCUMENT NUMBER: 107:3691
ORIGINAL REFERENCE NO.: 107:691a,694a
TITLE: Determination of antioxidative activity of chemical compounds
AUTHOR(S): Blagorodov, S. G.; Shepelev, A. P.; Dmitrieva, N. A.; Chernavskaya, L. N.; Koblik, A. V.; Suzdalev, K. F.; Kholodova, N. V.; Kuznetsov, E. V.; Bren, Zh. V.; et al.
CORPORATE SOURCE: Rostov. NII Epidemiol., Mikrobiol. Gig., Rostov-on-Don, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1987), 21(3), 292-4
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 107:3691
AB Ascorbate-dependent peroxidn. (aqueous oleic acid solution containing Tween 80) was used for determining antioxidant properties of various classes of compds. Malondialdehyde formation was monitored by the thiobarbituric acid test. Among the investigated compds., the cinnamaldehyde derivative cinnamal-p-amino-N,N,N-trimethylanilinium perchlorate and 4,6-diphenyl(3'-keto-[1,2,a]pyrazino)pyridinium perchlorate inhibited malondialdehyde formation by 30-70% compared to the control; other compds. increased malondialdehyde formation by 20-50%.
IT 69504-70-7P, 3-(3,4-Dimethoxyphenyl)-6,7-dimethoxyisoquinoline
RL: PREP (Preparation)
(preparation of, antioxidant property in relation to)
RN 69504-70-7 HCAPLUS
CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)

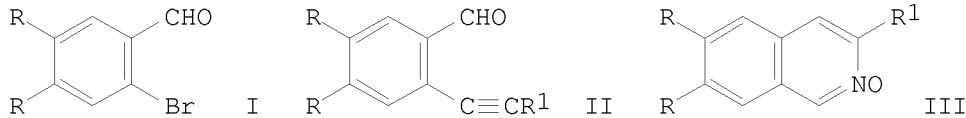


Updated Search

STN

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 140 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1987:84367 HCAPLUS
DOCUMENT NUMBER: 106:84367
ORIGINAL REFERENCE NO.: 106:13844h,13845a
TITLE: Condensed heteroaromatic ring systems. XI. A facile synthesis of isoquinoline N-oxides
Sakamoto, Takao; Kondo, Yoshinori; Miura, Norio;
Hayashi, Kazuhiko; Yamanaka, Hiroshi
Pharm. Inst., Tohoku Univ., Aobayama, 980, Japan
Heterocycles (1986), 24(8), 2311-14
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:84367
GI

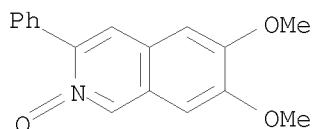


AB Treatment of bromobenzaldehydes I ($R = H, OMe$) with $R1C.tpbond.CH$ ($R1 = Ph, Bu, Me3Si$) in DMF 1-2 h at 40-50° in the presence of $Pd(PPh_3)_2Cl_2$, CuI , and Et_3N gave 66-88% six ethynylbenzaldehydes II (same R and $R1$), which were converted to the corresponding oximes (yields 80-99%), which on heating in $EtOH-H_2O-K_2CO_3$ at 60° for 1-5 h gave 35-78% isoquinoline oxides III (R same; $R1 = Ph, Bu, H$).

IT 106824-57-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 106824-57-1 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-3-phenyl-, 2-oxide (CA INDEX NAME)



OS.CITING REF COUNT: 33 THERE ARE 33 CAPLUS RECORDS THAT CITE THIS RECORD (34 CITINGS)

L13 ANSWER 141 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1986:583422 HCAPLUS
DOCUMENT NUMBER: 105:183422
ORIGINAL REFERENCE NO.: 105:29425a,29428a

STN

TITLE: Determination of pKa values of 2,2'-bipyridyl analogs and stability constants of their copper(I) and copper(II) complexes; relationship to antimycoplasmal activity

AUTHOR(S): Gaisser, H. D.; Van der Goot, H.; Timmerman, H.

CORPORATE SOURCE: Dep. Pharmacochem., Vrije Univ., Amsterdam, 1081 HV, Neth.

SOURCE: European Journal of Medicinal Chemistry (1986), 21(4), 285-9

CODEN: EJMCA5; ISSN: 0223-5234

DOCUMENT TYPE: Journal

LANGUAGE: English

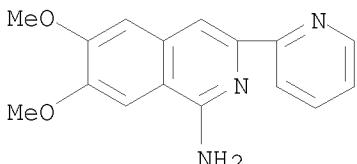
AB The stability consts. of Cu(I) and Cu(II) complexes of various 2,2'-bipyridyl analogs with potent antimycoplasmal activity were determined. Due to poor water solubility the measurements were carried out in a mixture of 50% dioxane/water. A good correlation between stability consts. of Cu(II) complexes and their pKa values, but not between the stability constant of Cu(I) complex and the stability consts. of Cu(II) complexes or the pKa of the ligands was observed. Although the antimycoplasmal effect of the investigated compds. strongly depends on the presence of Cu, their activity is not solely determined by one of the stability consts. Thus, the stability of the Cu(I) complex plays an important role.

IT 69767-44-8D, copper complexes

RL: PRP (Properties)
(formation and stability consts. of, antimycoplasmal activity in relation to)

RN 69767-44-8 HCPLUS

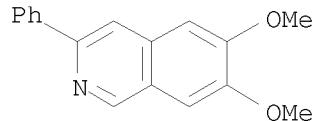
CN 1-Isoquinolinamine, 6,7-dimethoxy-3-(2-pyridinyl)- (CA INDEX NAME)



L13 ANSWER 142 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1986:514650 HCPLUS
DOCUMENT NUMBER: 105:114650
ORIGINAL REFERENCE NO.: 105:18546h, 18547a
TITLE: Effect of ethyl polyphosphate on N-acyl-1,2-diarylaminooethane
AUTHOR(S): Aguirre, J. M.; Alessio, E. N.; Somoza, C.; Tombari, D. G.; Moltrasio, G. Y.; Bonafede, J. D.
CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, 1113, Argent.
SOURCE: Anales de la Asociacion Quimica Argentina (1985), 73(4), 391-9
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

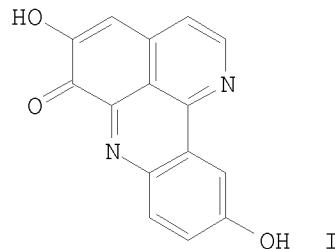
AB The reaction of acylaminodiarylethanes I (R = H, Ph; R1 = H, Me, Ph; R2-R5 = H, OMe) with tetra-Et cyclic metaphosphate gave stilbenes II, indans III, or isoquinolines IV depending on the substitution pattern of I.
 IT 104151-20-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 104151-20-4 HCPLUS
 CN Isoquinoline, 6,7-dimethoxy-3-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

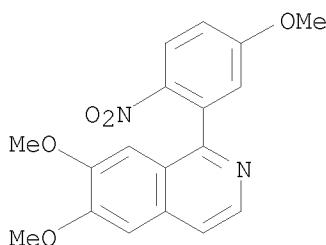
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
 (3 CITINGS)

L13 ANSWER 143 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1986:479209 HCPLUS
 DOCUMENT NUMBER: 105:79209
 ORIGINAL REFERENCE NO.: 105:12861a,12864a
 TITLE: Pigments of fungi. 48. Synthesis of necatorone
 AUTHOR(S): Hilger, Christoph Stephan; Fugmann, Burkhard;
 Steglich, Wolfgang
 CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300,
 Fed. Rep. Ger.
 SOURCE: Tetrahedron Letters (1985), 26(48), 5975-8
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:79209
 GI



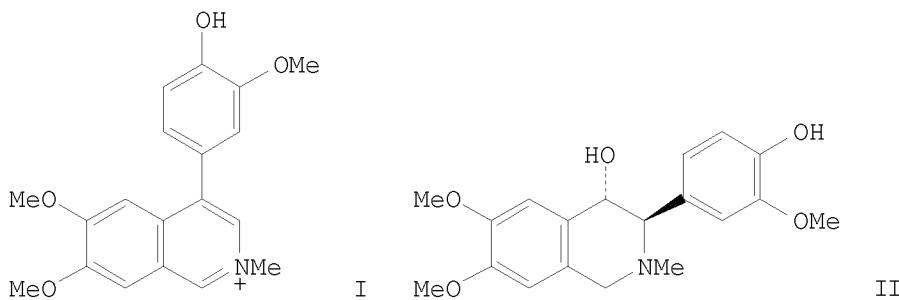
STN

AB The mutagenic fungal alkaloid necatorone (I) was obtained by a six-step synthesis starting from 2-(3,4-dimethoxyphenyl)ethylamine and 2-nitro-5-methoxybenzoyl chloride.
IT 103771-57-9
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)
RN 103771-57-9 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(5-methoxy-2-nitrophenyl)- (CA INDEX NAME)



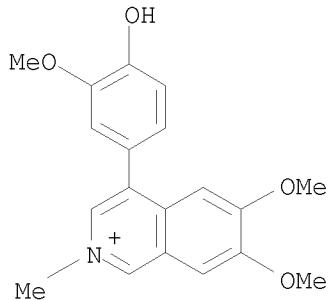
OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

L13 ANSWER 144 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1986:224821 HCAPLUS
DOCUMENT NUMBER: 104:224821
ORIGINAL REFERENCE NO.: 104:35659a,35662a
TITLE: The synthesis of a 4-phenylisoquinoline from a 3-phenylisoquinoline by utilization of a nitrogen analog of the pinacol rearrangement
Cushman, Mark; Mohan, Prem
AUTHOR(S): Sch. Pharm. Pharm. Sci., Purdue Univ., West Lafayette, IN, 47907, USA
CORPORATE SOURCE:
SOURCE: Tetrahedron Letters (1985), 26(38), 4563-6
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CODEN: TELEAY; ISSN: 0040-4039
GI: CASREACT 104:224821



STN

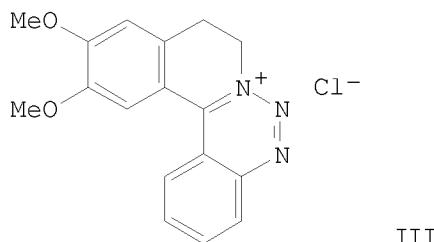
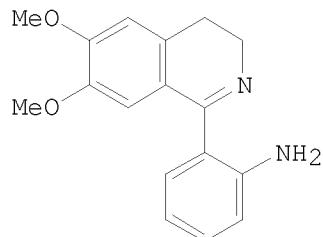
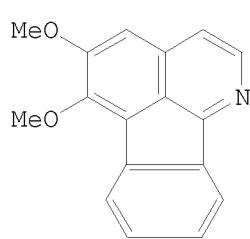
AB The nitrogen analog of the pinacol rearrangement was used for the preparation of a 4-phenylisoquinoline I from the intermediate amino alc. II.
IT 102349-19-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 102349-19-9 HCPLUS
CN Isoquinolinium, 4-(4-hydroxy-3-methoxyphenyl)-6,7-dimethoxy-2-methyl-, chloride (1:1) (CA INDEX NAME)



● Cl⁻

OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L13 ANSWER 145 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1986:149213 HCPLUS
DOCUMENT NUMBER: 104:149213
ORIGINAL REFERENCE NO.: 104:23637a, 23640a
TITLE: Azafluoranthene alkaloids: a reinvestigation of the synthesis of 5,6-dimethoxyindeno[1,2,3-ij]isoquinoline
Menachery, Mary D.; Buck, Keith T.
Chem. Dep., Pennsylvania State Univ., Altoona, PA,
16601-3760, USA
SOURCE: Heterocycles (1985), 23(10), 2677-9
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:149213
GI



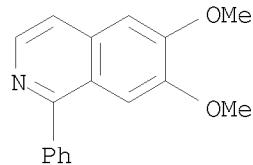
AB The title alkaloid (triclisine, I), was prepared by diazotization-cyclization of the isoquinoline II to give the benzotriazinium salt III, which underwent thermal decomposition followed by dehydrogenation.

IT 4029-09-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 4029-09-8 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 146 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1986:126391 HCAPLUS

DOCUMENT NUMBER: 104:126391

ORIGINAL REFERENCE NO.: 104:19923a, 19926a

TITLE: The influence of 2,2'-bipyridyl analogs on copper uptake by *Mycoplasma gallisepticum*

AUTHOR(S): Gaisser, H. Dieter; Van der Goot, Henk; Timmerman, Henk

CORPORATE SOURCE: Dep. Pharmacochem., Vrije Univ., Amsterdam, 1081 HV, Neth.

SOURCE: European Journal of Medicinal Chemistry (1985), 20(6), 513-15

CODEN: EJMCA5; ISSN: 0223-5234

STN

DOCUMENT TYPE: Journal
LANGUAGE: English

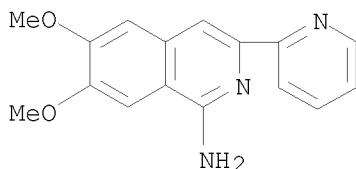
AB The uptake of Cu by *M. gallisepticum* cells was established in the presence of different concns. of a number of 2,2'-bipyridyl analogs. At their min. inhibitory concns., all 2,2'-bipyridyl analogs caused Cu uptake to the same level. In the absence of a 2,2'-bipyridyl derivative much more Cu has to be taken up by the cell for a growth inhibitory effect; this is probably due to a mechanism by which Cu is concentrated in the cell membrane.

IT 69767-44-8

RL: BIOL (Biological study)
(copper uptake by *Mycoplasma gallisepticum* stimulation by,
antimycoplasmal activity in relation to)

RN 69767-44-8 HCAPLUS

CN 1-Isoquinolinamine, 6,7-dimethoxy-3-(2-pyridinyl)- (CA INDEX NAME)



L13 ANSWER 147 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1986:69042 HCAPLUS

DOCUMENT NUMBER: 104:69042

ORIGINAL REFERENCE NO.: 104:11064h,11065a

TITLE: The structure of 2,3-dihydromenisperphine and the synthesis of dauriporphine, oxoisoaporphine alkaloids from *Menispernum dauricum* DC

AUTHOR(S): Kunitomo, Jun Ichi; Kaede, Sayuri; Satoh, Miyoko

CORPORATE SOURCE: Fac. Pharm. Sci., Mukogawa Women's Univ., Nishinomiya, 663, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(7), 2778-82

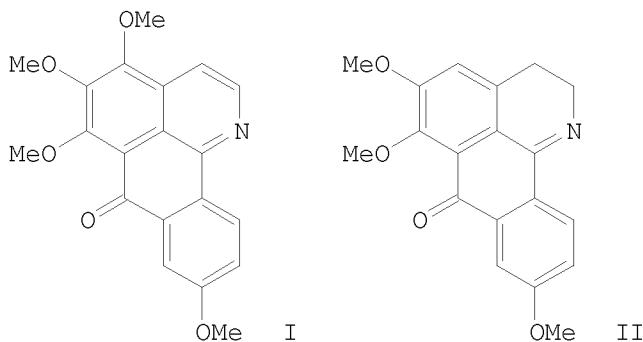
CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

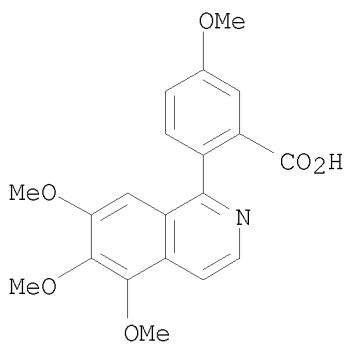
LANGUAGE: English

OTHER SOURCE(S): CASREACT 104:69042

GI



AB Two structurally unidentified alkaloids (tentatively named bases III and IV), isolated from *Menispermum dauricum* DC. (Menispermaceae), were found to be dauriporphine (I), a known oxoisoaporphine-type alkaloid, and 2,3-dihydromenisporphine (II), a new alkaloid of the same type, resp. The structure of dauriporphine was confirmed by synthesis of 4,5,6,9-tetramethoxy-7H-dibenzo[de,h]quinolin-7-one (I).
 IT 100009-77-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and esterification of)
 RN 100009-77-6 HCPLUS
 CN Benzoic acid, 5-methoxy-2-(5,6,7-trimethoxy-1-isoquinolinyl)- (CA INDEX NAME)

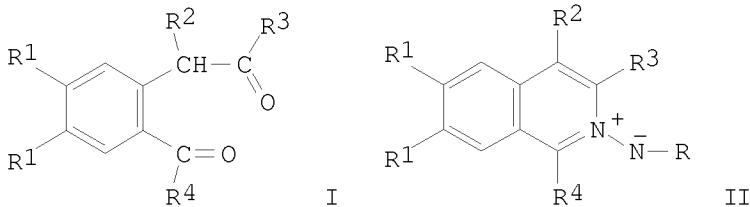


OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

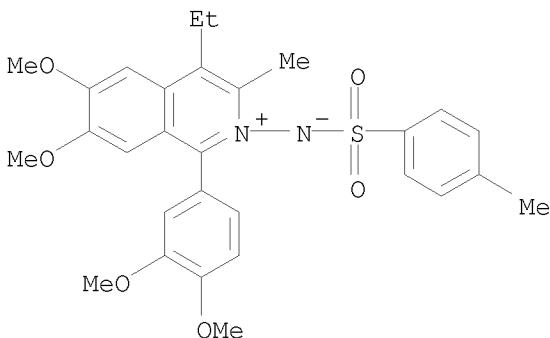
L13 ANSWER 148 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1985:560361 HCPLUS
 DOCUMENT NUMBER: 103:160361
 ORIGINAL REFERENCE NO.: 103:25737a, 25740a
 TITLE: The preparation of isoquinoline-N-imines by the reaction of 1-acyl-2-(2'-oxoalkyl)arenes with hydrazides
 AUTHOR(S): Anderson, Patrick N.; Sharp, John T.; Sood, H. Raj
 CORPORATE SOURCE: Dep. Chem., Univ. Edinburgh, Edinburgh, EH9 3JJ, UK

STN

SOURCE: *Synthesis* (1985), (1), 106-7
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:160361
GI



AB Cyclization of acyl(oxoalkyl)arenes I [R¹ = R² = R³ = R⁴ = H; R¹ = MeO, R² = Et, R³ = Me, R⁴ = 3,4-(MeO)₂C₆H₃] with RNHNH₂ (R = p-tosyl, PhSO₂, MeSO₂, Bz) gave 37-85% 6 isoquinoline-N-imines II.
IT 98352-06-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectrum of)
RN 98352-06-8 HCPLUS
CN Isoquinolinium, 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl-2-[(4-methylphenyl)sulfonyl]amino]-, inner salt (CA INDEX NAME)

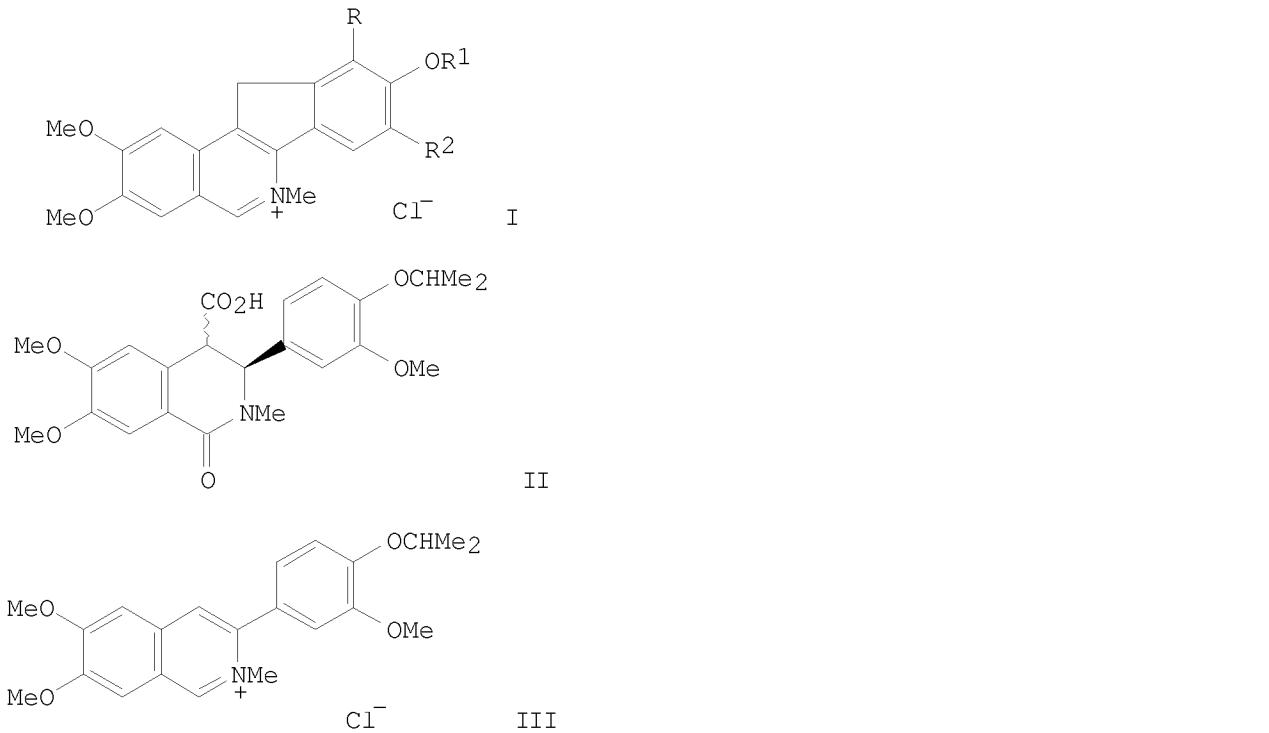


OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 149 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1985:437647 HCPLUS
DOCUMENT NUMBER: 103:37647
ORIGINAL REFERENCE NO.: 103:6115a,6118a
TITLE: Synthesis and antitumor activity of structural analogs of the anticancer benzophenanthridine alkaloid fagaronine chloride
AUTHOR(S): Cushman, Mark; Mohan, Prem
CORPORATE SOURCE: Sch. Pharm. Pharmacal Sci., Purdue Univ., West Lafayette, IN, 47907, USA

SOURCE: Journal of Medicinal Chemistry (1985),
 28(8), 1031-6
 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 103:37647
 GI



AB The indenoisoquinoline analog I ($R = R1 = H$, $R2 = MeO$) of fagaronine chloride was prepared, as well as its positional isomer I ($R = MeO$, $R1 = R2 = H$) and the corresponding mesylated derivs. were prepared from 3,4-MeO(Me₂CHO)C₆H₃CN:NMe via cyclization of isoquinolines II. Compds. I ($R = H$, $R1 = H$, MeSO, $R2 = MeO$; $R = MeO$, $R1 = R2 = H$) were tested against P388 lymphocytic leukemia and found to possess significant activity. A tricyclic analog III was also synthesized and was devoid of cytotoxicity in the KB cancer cell culture system. The change in the substitution pattern of the A-ring on going from I ($R = R1 = H$, $R2 = MeO$) to I ($R = MeO$, $R1 = R2 = H$) was tolerated without producing a significant decrease in antitumor activity.

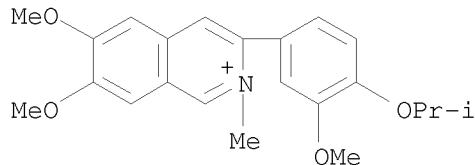
IT 96705-74-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antitumor activity of)

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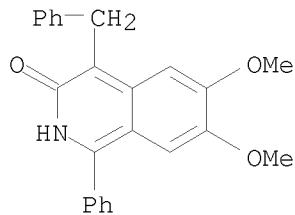
RN 96705-74-7 HCAPLUS
CN Isoquinolinium, 6,7-dimethoxy-3-[3-methoxy-4-(1-methylethoxy)phenyl]-2-methyl-, chloride (1:1) (CA INDEX NAME)



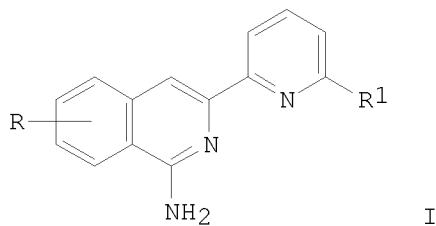
● Cl⁻

OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L13 ANSWER 150 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1985:166634 HCAPLUS
DOCUMENT NUMBER: 102:166634
ORIGINAL REFERENCE NO.: 102:26197a,26200a
TITLE: Diels-Alder reaction of 3(2H)-isoquinolinones, III.
Synthesis of adducts with maleic acid derivatives
AUTHOR(S): Hazai, L.; Schnitta, A.; Deak, G.; Toth, G.; Szollosy, A.
CORPORATE SOURCE: Inst. Exp. Med., Hung. Acad. Sci., Budapest, H-1450, Hung.
SOURCE: Acta Chimica Hungarica (1984), 117(1), 99-116
CODEN: ACHUDC; ISSN: 0231-3146
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:166634
AB A number of Diels-Alder adducts were synthesized by reacting 3(2H)-isoquinolinones with N-phenylmaleimide, maleic anhydride, and N-carbamoylmaleimide dienophiles. Adduct formation with isoquinolinones having an addnl. fused benzene ring were also examined. In some cases, when the starting 3(2H)-isoquinolinone could not be isolated as a pure compound, identification was achieved by means of the adduct obtained in the Diels-Alder reaction.
IT 87748-01-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(Diels-Alder reactions of, with maleic acid derivs.)
RN 87748-01-4 HCAPLUS
CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl-4-(phenylmethyl)- (CA INDEX NAME)



L13 ANSWER 151 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1985:166593 HCPLUS
 DOCUMENT NUMBER: 102:166593
 ORIGINAL REFERENCE NO.: 102:26189a, 26192a
 TITLE: Synthesis and antimycoplasmal activity of 2,2'-bipyridyl analogs. Part I.
 1-Amino-3-(2-pyridyl)isoquinolines
 AUTHOR(S): Pijper, Piet J.; Van der Goot, Henk; Timmerman, Henk;
 Nauta, Wijbe T.
 CORPORATE SOURCE: Dep. Pharmacochem., Vrije Univ., Amsterdam, 1081 HV,
 Neth.
 SOURCE: European Journal of Medicinal Chemistry (1984
), 19(5), 389-92
 CODEN: EJMCA5; ISSN: 0223-5234
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 102:166593
 GI



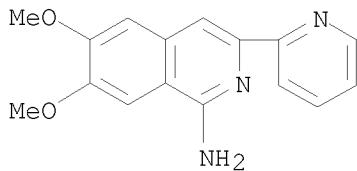
AB The pyridylisoquinolines I [R = H, Me, Cl, 7-, 8-Et, 6,7-(MeO)2, 6-Br, 7-iodo, R1 = H, R1 = Me, Et] were prepared by cyclocondensation of 2-methylbenzonitriles and 2-pyridinecarbonitriles. Min. inhibitory concns. of I against *Mycoplasma gallisepticum* in presence of Cu²⁺ were determined

IT 69767-44-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and antimycoplasmal activity of)

RN 69767-44-8 HCPLUS

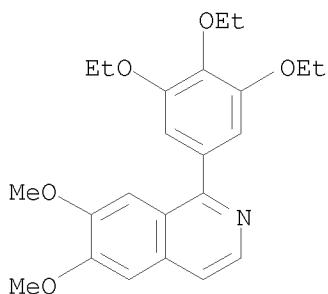
CN 1-Isoquinolinamine, 6,7-dimethoxy-3-(2-pyridinyl)- (CA INDEX NAME)

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OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 152 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1985:154850 HCAPLUS
DOCUMENT NUMBER: 102:154850
ORIGINAL REFERENCE NO.: 102:24281a,24284a
TITLE: Application of principal components analysis to TLC data for 596 basic and neutral drugs in four eluent systems
AUTHOR(S): Musumarra, Giuseppe; Scarlata, Giuseppe; Romano, Guido; Clementi, Sergio; Wold, Svante
CORPORATE SOURCE: Ist. Dip. Chim. Ind., Univ. Catania, Catania, 95125, Italy
SOURCE: Journal of Chromatographic Science (1984), 22(12), 538-47
CODEN: JCHSBZ; ISSN: 0021-9665
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Principal component anal. of the R_f values for 596 basic and neutral drugs in 4 eluent mixts. provided a significant 2-component model which explained 77% of the total variance. Each drug was characterized on a plane by 2 principal component scores. The loading plot shows that 3 eluent mixts. are clustered into the same group providing similar information. For identification of unknowns, the method provided a drastic reduction of the range of possibilities to a few candidates.
IT 549-68-8
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, thin-layer, principal component anal. in)
RN 549-68-8 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



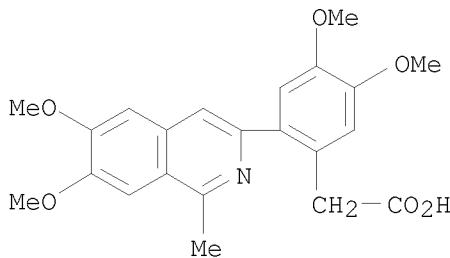
OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(9 CITINGS)

STN

L13 ANSWER 153 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1985:6891 HCAPLUS
DOCUMENT NUMBER: 102:6891
ORIGINAL REFERENCE NO.: 102:1251a,1254a
TITLE: Synthesis of some 3-arylisochromene,
3-arylisouquinoline, 6H-5-oxachrysene, and
benzo[c]phenanthridine analogs of some naturally
occurring alkaloids
AUTHOR(S): Carty, Antoine; Elliott, I. Wesley; Lenior, Grefonda
M.
CORPORATE SOURCE: Dep. Chem., Fisk Univ., Nashville, TN, 37203, USA
SOURCE: Canadian Journal of Chemistry (1984),
62(11), 2435-9
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A 2-benzopyrylium perchlorate I was prepared from the keto ester II. Reduction of I followed by dilute HCl affords 6H-5-oxachrysene III. Reaction of I with ammonia solution gives the isoquinoline acid IV. By a short series of steps IV is cyclized to the dihydrobenzo[c]phenanthridine V.
IT 93772-14-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and esterification of)
RN 93772-14-6 HCAPLUS
CN Benzeneacetic acid, 2-(6,7-dimethoxy-1-methyl-3-isoquinolinyl)-4,5-dimethoxy- (CA INDEX NAME)

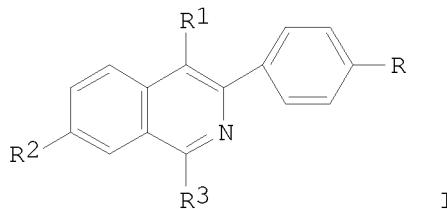


OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

L13 ANSWER 154 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1985:6157 HCAPLUS
DOCUMENT NUMBER: 102:6157
ORIGINAL REFERENCE NO.: 102:1115a,1118a
TITLE: Isoquinoline derivatives from the Ritter-type reaction
of vinyl cations

STN

AUTHOR(S): Kitamura, Tsugio; Kobayashi, Shinjiro; Taniguchi, Hiroshi
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Chemistry Letters (1984), (8), 1351-4
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:6157
GI



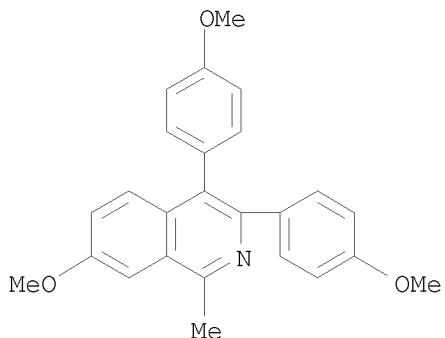
AB Both Ag-assisted reaction of 4-R₂C₆H₄CR₁:CBrC₆H₄R-4 (R = H, MeO:Me; R₁ = Ph, 4-MeOC₆H₄; R₂ = H, OMe) and their photolysis in R₃CN (R₃ = Me, Et, Ph) gave isoquinoline I, indicating that a Ritter reaction involving a vinyl cation took place.

IT 93472-43-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from arylvinyl bromide and nitrile)

RN 93472-43-6 HCPLUS

CN Isoquinoline, 7-methoxy-3,4-bis(4-methoxyphenyl)-1-methyl- (CA INDEX NAME)

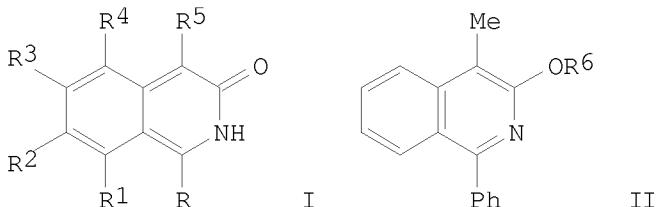


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L13 ANSWER 155 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:610946 HCPLUS
DOCUMENT NUMBER: 101:210946
ORIGINAL REFERENCE NO.: 101:31959a,31962a
TITLE: Diels-Alder reaction of 3(2H)-isoquinolinones, II.
Studies on the lactam-lactim tautomerism of

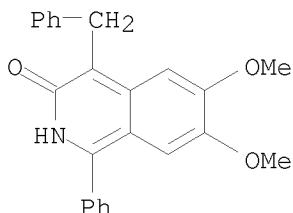
STN

AUTHOR(S): 3(2H)-isoquinolinones
Hazai, L.; Deak, G.; Schnitta, A.; Hasko-Breuer, J.;
Horvath, E.
CORPORATE SOURCE: Inst. Exp. Med., Hung. Acad. Sci., Budapest, H-1450,
Hung.
SOURCE: Acta Chimica Hungarica (1984), 116(3),
303-13
DOCUMENT TYPE: CODEN: ACHUDC; ISSN: 0231-3146
Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:210946
GI



AB UV and IR spectra were used to determine the lactam-lactim isomerism in isoquinolinones I (R = Ph, 4-ClC₆H₄, 4-pyridyl, 3-pyridyl, 4-AcNH₂C₆H₄; R₁ = H; R₂ = H, OMe; R₁R₂, R₃R₄ = CH:CHCH:CH; R₃ = H, OMe; R₄ = H, Me; R₅ = Me, CH₂Ph, 4-pyridyl, 3-pyridyl, H) and related compds. In EtOH the isoquinolinones occur mainly in the lactam form, whereas benzisoquinolines occur predominantly in the lactam form. I (R = Ph, R₁ = R₄ = H, R₂ = R₃ = OMe, R₅ = CH₂Ph; R = 4-pyridyl, R₁-R₄ = H, R₅ = H, 3-pyridyl) and the lactims II (R₆ = allyl, SO₂Me) were prepared

IT 87748-01-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and lactam-lactim tautomerism in, UV and IR spectra in relation to)
RN 87748-01-4 HCPLUS
CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl-4-(phenylmethyl)- (CA INDEX NAME)

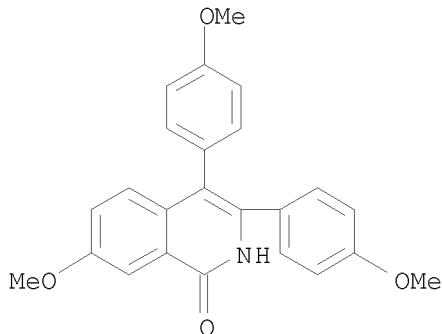


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 156 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:610488 HCPLUS

STN

DOCUMENT NUMBER: 101:210488
ORIGINAL REFERENCE NO.: 101:31882h, 31883a
TITLE: Reaction of photogenerated vinyl cations with ambident anions
AUTHOR(S): Kitamura, Tsugio; Kobayashi, Shinjiro; Taniguchi, Hiroshi
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Hakozaki, 812, Japan
SOURCE: Chemistry Letters (1984), (9), 1523-6
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:210488
AB Photolysis of vinyl bromides with cyanate anion in a two-phase system gave only isoquinolinones as the N-site attacked products. However, the photolysis with thiocyanate anion gave both the N-site attacked products, isothioquinolinones or vinyl isothiocyanates, and the S-site attacked products, vinyl thiocyanates.
IT 93119-93-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by photolysis of vinyl bromides in presence of cyanate anion)
RN 93119-93-8 HCAPLUS
CN 1(2H)-Isoquinolinone, 7-methoxy-3,4-bis(4-methoxyphenyl)- (CA INDEX NAME)

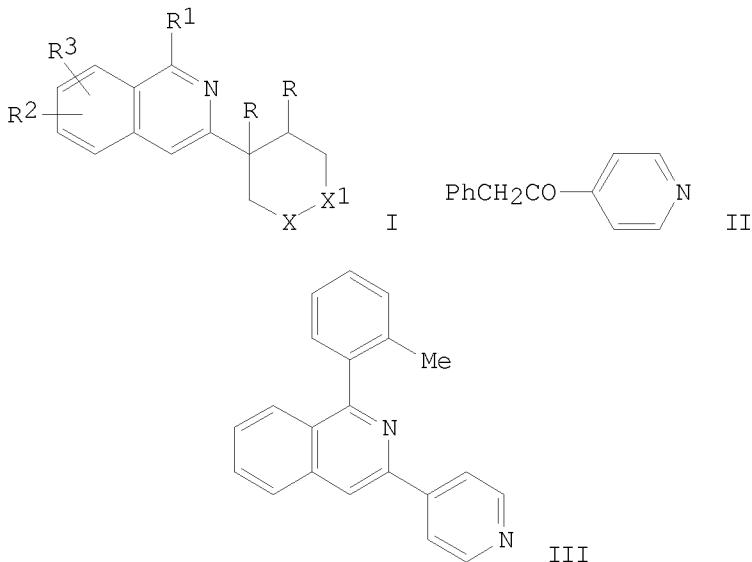


OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

L13 ANSWER 157 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:551766 HCAPLUS
DOCUMENT NUMBER: 101:151766
ORIGINAL REFERENCE NO.: 101:22971a, 22974a
TITLE: 1-Phenylisoquinoline derivatives useful in treating the central nervous system, especially as antidepressants
INVENTOR(S): Konz, Elmar; Kruse, Hansjoerg
PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 27 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3244594	A1	19840607	DE 1982-3244594	19821202 <--
EP 110372	A1	19840613	EP 1983-111922	19831129 <--
EP 110372	B1	19860910		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 22077	T	19860915	AT 1983-111922	19831129 <--
US 4547508	A	19851015	US 1983-556684	19831130 <--
JP 59110691	A	19840626	JP 1983-225528	19831201 <--
PRIORITY APPLN. INFO.:			DE 1982-3244594	A 19821202
			EP 1983-111922	A 19831129
OTHER SOURCE(S):	CASREACT 101:151766; MARPAT 101:151766			
GI				



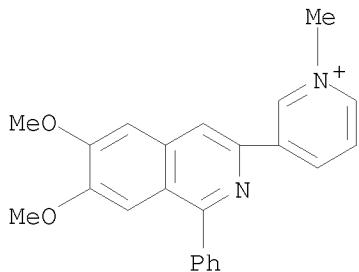
AB The title compds. [I; R = H, R2 = bond; R1 = (un)substituted Ph, R2, R3 = H, alkyl, alkoxy, amino, PhCH₂O, OH, NO₂, halo; R2R3 = OCH₂O, OCH₂CH₂O; X, X1 = CH₂, R4N; R4 = H, alkyl, alkenyl] were prepared. Thus, 4-pyridinecarbonitrile underwent a Grignard reaction with PhCH₂Cl to give, after hydrolysis, benzyl pyridyl ketone II. This was oxidized, reduced to the amine, benzoylated with 2-MeC₆H₄COCl, and cyclized with P₂O₅ to give pyridylisoquinoline III. This was quaternized with EtI and reduced with NaBH₄ to give I (R2 = bond, R1 = 2-MeC₆H₄, R2 = R3 = H, X = CH, X1 = NH) (IV). In mice IV inhibited tetrabenazine-induced ptosis with an ED₅₀ of 1.4 mg/kg i.p.

IT 92124-21-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and borohydride reduction of)

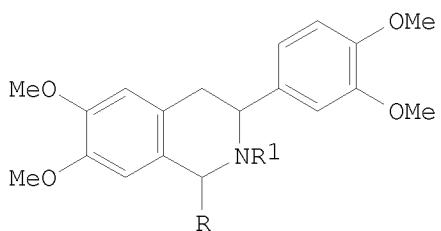
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RN 92124-21-5 HCAPLUS
CN Pyridinium, 3-(6,7-dimethoxy-1-phenyl-3-isoquinolinyl)-1-methyl-, iodide
(1:1) (CA INDEX NAME)



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L13 ANSWER 158 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:490742 HCAPLUS
DOCUMENT NUMBER: 101:90742
ORIGINAL REFERENCE NO.: 101:13907a, 13910a
TITLE: Dehydrogenation reactions of
1-substituted-3-aryltetrahydroisoquinoline derivatives
AUTHOR(S): Dominguez, Esther; Lete, Esther
CORPORATE SOURCE: Fac. Cienc., Univ. Pais Vasco, Bilbao, Spain
SOURCE: Journal of Heterocyclic Chemistry (1984),
21(2), 525-8
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:90742
GI

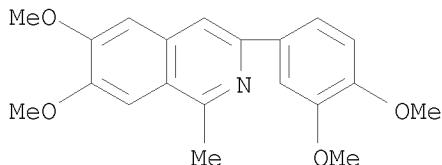


I

AB The title compds. I (R = H, Me, Ph, 3,4-(MeO)₂C₆H₃; R¹ = H, Me) were converted into the corresponding 3,4-dihydro- or isoquinoline derivs. by treatment with several oxidizing agents: iodine in ethanol, Pd/C, DDQ and Fremy's salt. The oxidation reactions with iodine always resulted in the formation of the 3,4-dihydroisoquinolines, whereas the use of Pd/C and the DDQ led to the aromatic isoquinolines. Both the 3,4-dihydro- and the

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isoquinoline derivs. were obtained by means of Fremy's salt.
IT 35989-93-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35989-93-6 HCAPLUS
CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



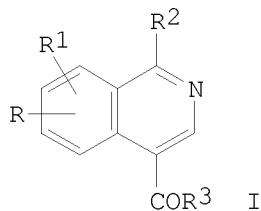
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 159 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:438362 HCAPLUS
DOCUMENT NUMBER: 101:38362
ORIGINAL REFERENCE NO.: 101:5993a,5996a
TITLE: Isoquinoline derivatives, pharmaceutical preparations from these compounds, and their use
INVENTOR(S): Konz, Elmar; Kaiser, Joachim
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 28 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3233424	A1	19840315	DE 1982-3233424	19820909 <--
EP 105210	A2	19840411	EP 1983-108697	19830903 <--
EP 105210	A3	19841010		
EP 105210	B1	19870304		
R: AT, BE, CH, FI, US, DK, NO, AU, JP, ZA, HU, CA	DE, FR, GB, IT, LI, LU, NL, SE			
AT 25679	T	19870315	AT 1983-108697	19830903 <--
FI 8303200	A	19840310	FI 1983-3200	19830907 <--
US 4673682	A	19870616	US 1983-530000	19830907 <--
DK 8304080	A	19840310	DK 1983-4080	19830908 <--
NO 8303217	A	19840312	NO 1983-3217	19830908 <--
AU 8318916	A	19840315	AU 1983-18916	19830908 <--
JP 59067270	A	19840416	JP 1983-164274	19830908 <--
ZA 8306663	A	19840425	ZA 1983-6663	19830908 <--
HU 32353	A2	19840730	HU 1983-3134	19830908 <--
HU 191094	B	19870128		
CA 1211445	A1	19860916	CA 1983-436316	19830908 <--
PRIORITY APPLN. INFO.:			DE 1982-3233424	A 19820909
			EP 1983-108697	A 19830903
OTHER SOURCE(S):	CASREACT 101:38362; MARPAT 101:38362			

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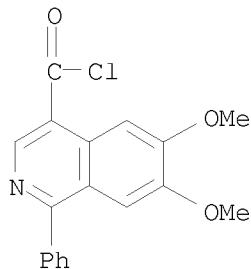
AB Isoquinolines I [R = H; R1 = H, alkyl, alkoxy, PhCH₂O, OH, NO₂, amino, halo; RR1 = OCH₂O, OCH₂CH₂O; R2 = (un)substituted Ph; R3 = OH, SH, alkoxy, alkylthio, R₄R₅Z; R₄, R₅ = H, alkyl; R₄R₅N = heterocyclyl; Z = alkylene, bond], having antiarrhythmic activity, were prepared. Thus, 3-chloro-1-(2-methylphenyl)-4-isooquinolinecarboxylic acid was dechlorinated by hydrogenation over Pd/C, converted to its acid chloride, and treated with Et₂NCH₂CH₂NH₂ to give I (R = R₁ = H, R₂ = 2-MeC₆H₄, R₃ = Et₂NCH₂CH₂NH).

IT 90829-21-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of diethylethanediamine)

RN 90829-21-3 HCPLUS

CN 4-Isoquinolinecarbonyl chloride, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 160 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1984:435051 HCPLUS

DOCUMENT NUMBER: 101:35051

ORIGINAL REFERENCE NO.: 101:5433a, 5436a

TITLE: 1-(4-Aminophenyl)isoquinoline derivatives. Potent
inhibitors of calcium-independent and
calcium-dependent phosphodiesterases from rat cerebral
cortex

AUTHOR(S): Davis, Craig W.; Walker, Kathleen A.

CORPORATE SOURCE: Sch. Med., Univ. South Carolina, Columbia, SC, 29208,
USA

SOURCE: Biochemical Pharmacology (1984), 33(8),
1205-12

CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal

STN

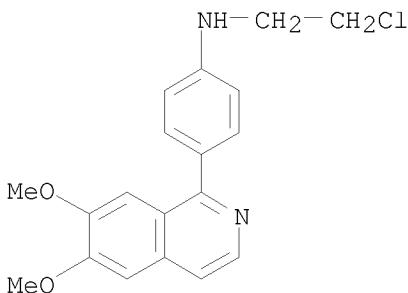
LANGUAGE: English
AB The effects of a series of 1-(4-aminophenyl)isoquinoline derivs. on the activity of Ca²⁺-independent and Ca²⁺-dependent cyclic nucleotide phosphodiesterases purified from rat cerebral cortex were examined. The agents were approx. equipotent (IC₅₀ (50% inhibitory concentration) values, 0.2-25 μM) in inhibiting the Ca²⁺-dependent hydrolysis of either cAMP or cGMP, whereas they were 6-35 -fold more effective as inhibitors of cAMP hydrolysis when compared to cGMP hydrolysis using the Ca²⁺-independent enzyme. The diastereomers of 3-(carbomethoxy)propenamido demonstrated a marked difference in specificity. The cis isomer was very potent in inhibiting cAMP or cGMP hydrolysis by either enzyme (IC₅₀ values, 0.2-8 μM), whereas the trans isomer was only effective in inhibiting Ca²⁺-independent cAMP hydrolysis (IC₅₀ values, 2.5 μM). Kinetic analyses of the type of inhibition of the Ca²⁺-dependent enzyme revealed that the various agents were competitive inhibitors of cGMP hydrolysis and noncompetitive inhibitors of cAMP hydrolysis. A reverse pattern of inhibition by the isoquinoline derivs. was found using the Ca²⁺-independent phosphodiesterase, i.e., noncompetitive inhibition of cGMP but competitive inhibition of cAMP. Inhibition of phosphodiesterases by these agents was also manifested using intact brain slices prepared from rat cerebral cortex. Thus, the agents potentiate forskolin-elicited accumulations of cAMP by 100-700% and increase the half-time for the decline in cAMP following forskolin stimulation from 3-6 min.

IT 83633-21-0

RL: BIOL (Biological study)
(cyclic nucleotide phosphodiesterase multiple forms of brain cerebral cortex inhibition by)

RN 83633-21-0 HCPLUS

CN Benzenamine, N-(2-chloroethyl)-4-(6,7-dimethoxy-1-isoquinolinyl)-(CA INDEX NAME)



L13 ANSWER 161 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1984:174683 HCPLUS

DOCUMENT NUMBER: 100:174683

ORIGINAL REFERENCE NO.: 100:26565a, 26568a

TITLE: 1-Phenylisoquinoline derivatives

TITLE: 1-Phenyl-1-isopropylidene-2-propanone
INVENTOR(S): Konz, Elma

INVENTOR(S): RÖHL, EIKAR, KRÄSE, HANS-JOERG, NECK, FRANZ
PATENT ASSIGNEE(S): HOECHST A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen. - 24 pp.

SOURCE: SER. ORIGIN., 21 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

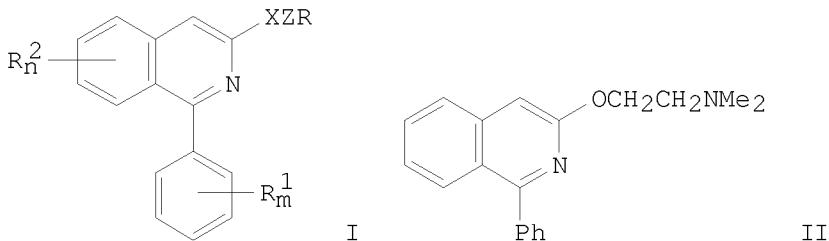
DOCUMENT TYPE: Facsimile
LANGUAGE: German

LANGUAGE : German

STN

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3227741	A1	19840126	DE 1982-3227741 DE 1982-3227741	19820724 <-- 19820724
PRIORITY APPLN. INFO.:			CASREACT 100:174683; MARPAT 100:174683	
OTHER SOURCE(S):				
GI				



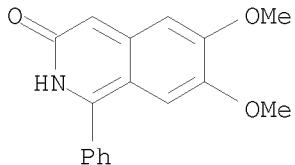
AB Title compds. (I) [X = O or S; m, n = 0-2; Z = bond or (un)substituted C1-8 alkylene; R = (un)substituted amino or N heterocycll; R1 = H, halo, OH, NO2, NH2, C1-6 alkyl or alkoxy; R2 = H, halo, OH, NH2, NO2, C1-6 alkyl or alkoxy, benzyloxy, OCH2O, OCH2CH2O] were prepared and shown to have antidepressant activity. Thus, 6.6 g 1-phenyl-3-isoquinolinol, 2.16 g 50% NaH, and 150 mL PhMe were stirred 1 h at 60°, cooled to 20°, treated dropwise with 5.3 g Me2NCH2CH2Cl, and stirred 2 h at 100° to give the isoquinolyl ether II.

IT 89721-03-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of, with (dimethylamino)ethyl chloride)

RN 89721-03-9 HCPLUS

CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 162 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:138972 HCPLUS
DOCUMENT NUMBER: 100:138972
ORIGINAL REFERENCE NO.: 100:21206h, 21207a
TITLE: Arene- and heteroarenecarboxamides
INVENTOR(S): Dubroeucq, Marie Christine; Renault, Christian; Le Fur, Gerard

STN

PATENT ASSIGNEE(S): Pharmuka Laboratoires, Fr.
SOURCE: Fr. Demande, 25 pp.

CODEN: FRXXBL

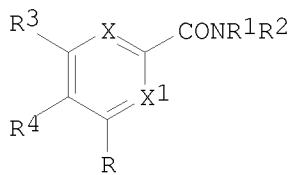
DOCUMENT TYPE: Patent

LANGUAGE: French

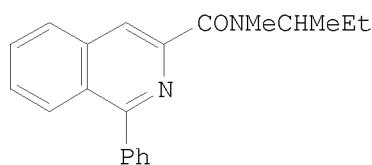
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2525595	A1	19831028	FR 1982-7217	19820427 <--
FR 2525595	B1	19850322		
US 4499094	A	19850212	US 1983-482082	19830405 <--
CA 1207324	A1	19860708	CA 1983-425918	19830414 <--
EP 94271	A2	19831116	EP 1983-400749	19830415 <--
EP 94271	A3	19840704		
EP 94271	B1	19860806		
R: BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 8301423	A	19861115	AT 1983-1423	19830420 <--
AT 383347	B	19870625		
DK 8301847	A	19831028	DK 1983-1847	19830426 <--
NO 8301466	A	19831028	NO 1983-1466	19830426 <--
JP 58201756	A	19831124	JP 1983-73653	19830426 <--
JP 03024467	B	19910403		
ZA 8302925	A	19840125	ZA 1983-2925	19830426 <--
HU 31662	A2	19840528	HU 1983-1431	19830426 <--
HU 189271	B	19860630		
AU 8314002	A	19831103	AU 1983-14002	19830427 <--
AU 555417	B2	19860925		
PRIORITY APPLN. INFO.:		FR 1982-7217		A 19820427
OTHER SOURCE(S):		CASREACT 100:138972; MARPAT 100:138972		
GI				



I



II

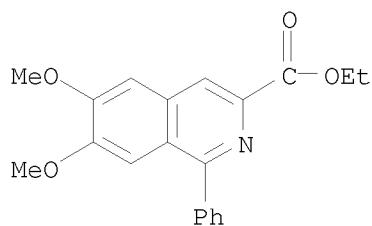
AB Carboxamides I [X, X1 = N, CH; R = Ph, substituted Ph, pyridyl, thienyl; R1, R2 = aliphatic, aromatic; NR1R2 = heterocyclic; R3R4 = (un)substituted CH:CHCH:CH, SCH:CH, CH:CHS] were prepared. Thus 2.4 g II was obtained by amidating 2.96 g of acid with 1.34 g MeNHCHMeEt. II had an affinity for benzodiazepine receptors of 2 nM.

IT 89242-43-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of)

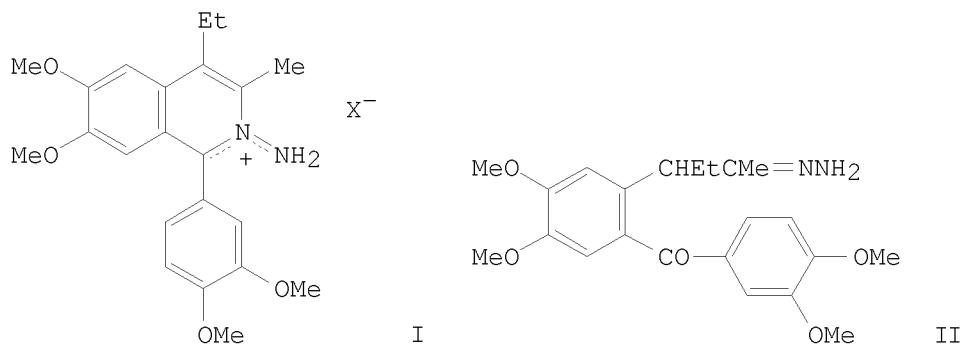
RN 89242-43-3 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-phenyl-, ethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
 (4 CITINGS)
 REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

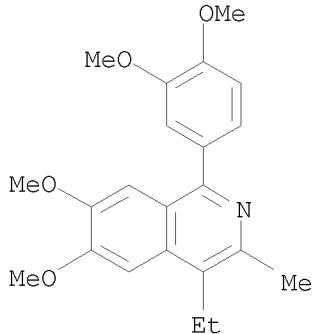
L13 ANSWER 163 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1984:103152 HCAPLUS
 DOCUMENT NUMBER: 100:103152
 ORIGINAL REFERENCE NO.: 100:15669a,15672a
 TITLE: Heterocyclic compounds. V. The preparation and characterization of 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-4-ethyl-3-methylisoquinoline-N-imine salts
 AUTHOR(S): Korosi, J.; Lang, T.; Neszmelyi, A.; Horvath, G.
 CORPORATE SOURCE: Inst. Drug Res., Budapest, H-1045, Hung.
 SOURCE: Acta Chimica Hungarica (1983), 114(3-4), 301-7
 DOCUMENT TYPE: CODEN: ACHUDC; ISSN: 0231-3146
 LANGUAGE: Journal
 OTHER SOURCE(S): English
 GI



AB The title compds. I [X = acetate, (R,R)-hydrogen tartrate, isopropyl sulfate, Cl] were prepared by cyclizing hydrazones II in the presence of the corresponding acid. I (X = Cl) was converted to I (X = HSO4, ClO4, SCN, HCO3, N3, HCrO4, FeCl4).
 IT 1616-49-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

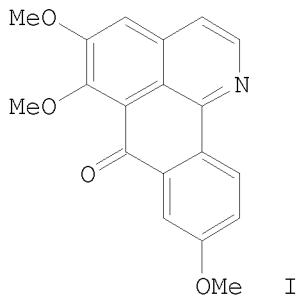
STN

RN 1616-49-5 HCAPLUS
CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl- (CA
INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPIUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 164 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:85966 HCAPLUS
DOCUMENT NUMBER: 100:85966
ORIGINAL REFERENCE NO.: 100:13041a,13044a
TITLE: Studies on the alkaloids of menispermaceous plants.
279. Alkaloids of Menispermum dauricum DC. 9.
Structure and synthesis of menisporphine, a new type
of isoquinoline alkaloid
AUTHOR(S): Kunitomo, J.; Satoh, M.; Shingu, T.
CORPORATE SOURCE: Fac. Pharm. Sci., Mukogawa Women's Univ., Nishinomiya,
663, Japan
SOURCE: Tetrahedron (1983), 39(20), 3261-5
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The structure of a yellow base from Menispermum dauricum DC.
(Menispermaceae) was determined to be the dibenzoquinolinone I from spectral
data and synthesis, and was named menisporphine. This is a new

STN

isoquinoline-type alkaloid having a 7H-dibenzo[de,h]quinolin-7-one skeleton for which the general term "oxoisoaporphine" is proposed.

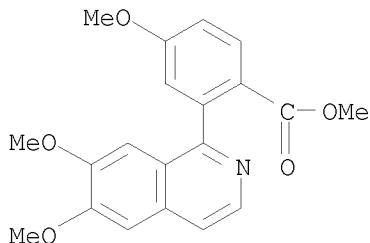
IT 88741-64-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, dibenzoquinolinone derivative from)

RN 88741-64-4 HCAPLUS

CN Benzoic acid, 2-(6,7-dimethoxy-1-isoquinolinyl)-4-methoxy-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

L13 ANSWER 165 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1983:594836 HCAPLUS

DOCUMENT NUMBER: 99:194836

ORIGINAL REFERENCE NO.: 99:29991a,29994a

TITLE: Diels-Alder reaction of 3(2H)-isoquinolinones. I

AUTHOR(S): Hazai, L.; Deak, G.; Toth, G.; Schnitta, A.; Szollosty, A.; Tamas, J.

CORPORATE SOURCE: Inst. Exp. Med., Hung. Acad. Sci., Budapest, H-1450, Hung.

SOURCE: Acta Chimica Hungarica (1983), 113(3), 237-41

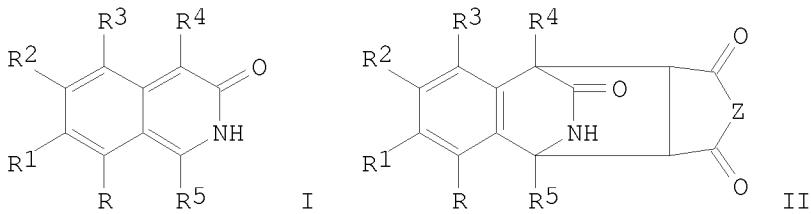
CODEN: ACHUDC; ISSN: 0231-3146

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:194836

GI



AB Isoquinolinones I (one of RR1, R1R2, and R2R3 is benzo while the remainder are H; or R = H, R1 = H or Me, R2 = H or OMe, and R3 = H or Me; R4 = Me, H, Ph, CHMe2, PhCH2, pyridylmethyl; R5 = Ph, 4-ClC6H4, pyridyl) were

STN

converted to adducts II ($Z = \text{NPh}, \text{O}$). I ($\text{R} = \text{R1} = \text{R2} = \text{R3} = \text{H}, \text{R4} = \text{Me}, \text{R5} = \text{Ph}$) was heated with excess N-phenylmaleimide in xylene to give II ($\text{R} = \text{R1} = \text{R2} = \text{R3} = \text{H}, \text{R4} = \text{Me}, \text{R5} = \text{Ph}, \text{Z} = \text{NPh}$).

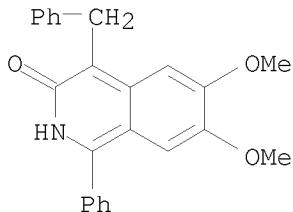
IT 87748-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(Diels-Alder reaction of, with maleimide derivative and maleic anhydride)

RN 87748-01-4 HCPLUS

CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl-4-(phenylmethyl)- (CA INDEX NAME)



L13 ANSWER 166 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1983:405445 HCPLUS

DOCUMENT NUMBER: 99:5445

ORIGINAL REFERENCE NO.: 99:989a,992a

TITLE: Nickel-phosphine complex-catalyzed Grignard coupling.
II. Grignard coupling of heterocyclic compounds

AUTHOR(S): Tamao, K.; Kodama, S.; Nakajima, I.; Kumada, M.;
Minato, A.; Suzuki, K.

CORPORATE SOURCE: Dep. Synth. Chem., Kyoto Univ., Kyoto, 606, Japan

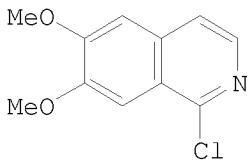
SOURCE: Tetrahedron (1982), 38(22), 3347-54

CODEN: TETRAB; ISSN: 0040-4020

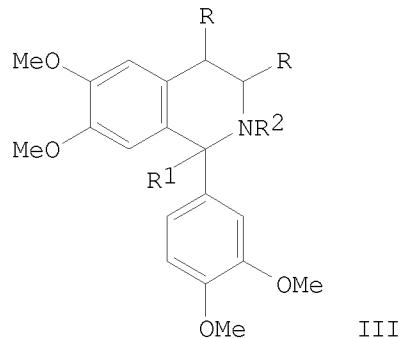
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



II



III

AB The alkylation and arylation of haloheterocyclic compds. by Grignard

Updated Search

STN

reagents was catalyzed by [NiCl₂L] [L = (Ph₂PCH₂)₂CH₂] (I). E.g., alkylation of 2-bromopyridine with BuMgBr in Et₂O containing I at room temperature

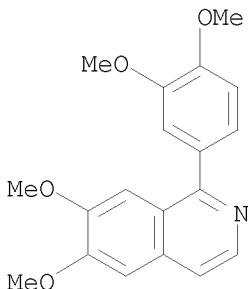
for 2.5 h gave 71% 2-butylpyridine. This coupling reaction was used in the preparation of alkaloids. E.g., coupling reaction of isoquinoline II with 3,4-(MeO)₂C₆H₃MgBr in the presence of I gave 66% isoquinoline III (R₂ = R₁R₂ = bond), a precursor of cryptostyline II (III; R = R₁ = H, R₂ = Me).

IT 15547-50-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by coupling reaction of haloisoquinoline with Grignard's reagent)

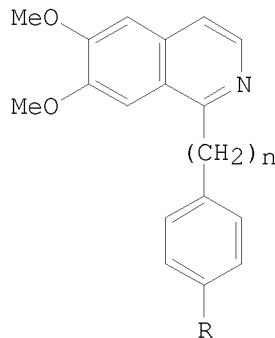
RN 15547-50-9 HCPLUS

CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 282 THERE ARE 282 CAPLUS RECORDS THAT CITE THIS RECORD (284 CITINGS)

L13 ANSWER 167 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1983:54262 HCPLUS
DOCUMENT NUMBER: 98:54262
ORIGINAL REFERENCE NO.: 98:8361a,8364a
TITLE: 1-(4-Aminobenzyl)- and 1-(4-aminophenyl)isoquinoline derivatives: synthesis and evaluation as potential irreversible cyclic nucleotide phosphodiesterase inhibitors
AUTHOR(S): Walker, Kathleen A.; Boots, Marvin R.; Stubbins, James F.; Rogers, Michael E.; Davis, Craig W.
CORPORATE SOURCE: Dep. Pharm. Chem., Virginia Commonw. Univ., Richmond, VA, 23298, USA
SOURCE: Journal of Medicinal Chemistry (1983), 26(2), 174-81
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



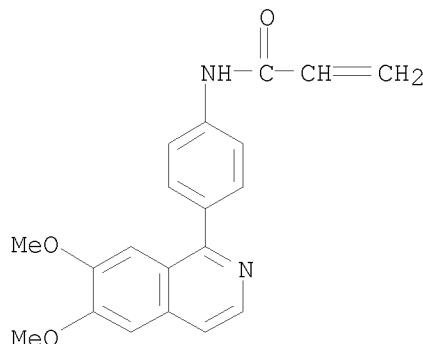
AB In an effort to increase the specificity of the potent phosphodiesterase inhibitor papaverine, two series of novel 1-(4-aminobenzyl)- and 1-(4-aminophenyl)isoquinoline derivs., I ($n = 0, 1$; $R = H_2N, NHCH_2CH_2Cl, N(CH_2CH_2Cl)_2, NHCOCH:CHCO_2Me, HNCOCH:CH_2$) were prepared. Thus $3,4-(MeO)_2C_6H_3CH_2CH_2NH_2$ was treated with $p-O_2NC_6H_4COCl$ followed by cyclization, dehydrogenation, and reduction to give I ($n = 0, R = NH_2$), which was treated with $H_2C:CHCOCl$ to give I ($n = 0, R = NHCOCH:CH_2$). These compds. were evaluated for their inhibitory action on phosphodiesterase preps. from bovine heart and rat cerebral cortex. Studies were also conducted to determine whether these compds. were reacting with the enzymes in an irreversible manner. The compds. were potent inhibitors of the phosphodiesterases; however, no evidence was found for an irreversible inhibition.

IT 83633-14-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phosphodiesterase inhibition activity of)

RN 83633-14-1 HCPLUS

CN 2-Propenamide, N-[4-(6,7-dimethoxy-1-isoquinolinyl)phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

L13 ANSWER 168 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1983:34818 HCPLUS
DOCUMENT NUMBER: 98:34818

STN

ORIGINAL REFERENCE NO.: 98:5456h,5457a

TITLE:

Hofmann degradation of β -hydroxy ammonium salts.

α - and β -Hydroxylaudanosine,

7-hydroxyglaucine, and 13-hydroxyxylopinine

AUTHOR(S):

Wert, Kathleen L.; Chackalamannil, Samuel; Miller, Eric; Dalton, David R.; Zacharias, David E.; Glusker, Jenny P.

CORPORATE SOURCE:

Dep. Chem., Temple Univ., Philadelphia, PA, 19122, USA

SOURCE:

Journal of Organic Chemistry (1982), 47(26),

5141-50

CODEN: JOCEAH; ISSN: 0022-3263

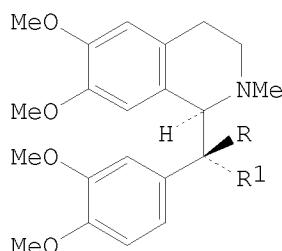
DOCUMENT TYPE:

Journal

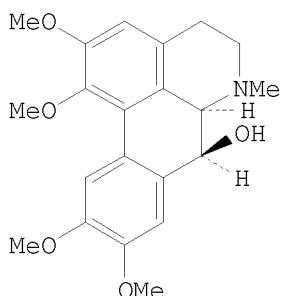
LANGUAGE:

English

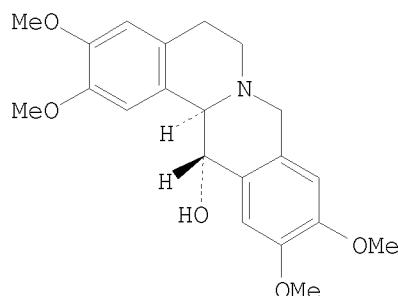
GI



I



II



III

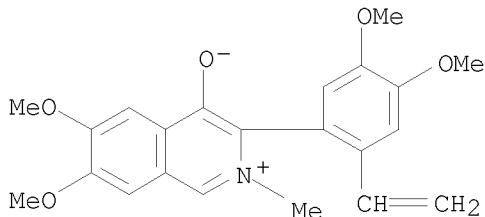
AB The four related β -hydroxy ammonium methiodide salts of β -hydroxylaudanosine (I, R = H, R1 = HO), β -hydroxylaudanosine (I, R = HO, R1 = H), 7-hydroxyglaucine (II), and 13-hydroxyxylopinine (III) were subjected to Hofmann degradation. Although precedent dictates that such materials should form either epoxides or ketones, these are not found. Only products of (a) fragmentation and elimination (from I), (b) dehydration and elimination (from II), and (c) elimination and oxidation (from III) are obtained. The results are accounted for by consideration of the mol. geometries of the β -hydroxy ammonium salts as exptl. determined from single-crystal x-ray studies and the geometric requirements for epoxide and ketone formation.

IT 83511-47-1P

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from Hofmann degradation of hydroxyxylopinine)

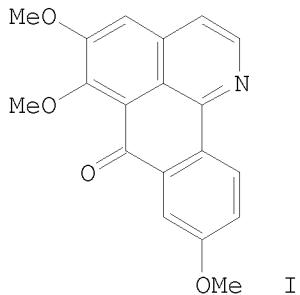
RN 83511-47-1 HCPLUS

CN Isoquinolinium, 3-(2-ethenyl-4,5-dimethoxyphenyl)-4-hydroxy-6,7-dimethoxy-2-methyl-, inner salt (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

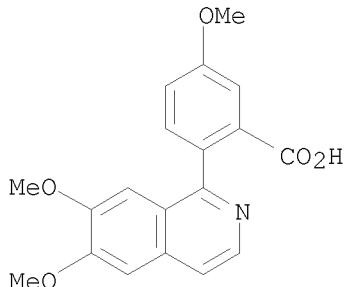
L13 ANSWER 169 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:598422 HCAPLUS
DOCUMENT NUMBER: 97:198422
ORIGINAL REFERENCE NO.: 97:33240h,33241a
TITLE: Structure of menisporphine: a new type of isoquinoline alkaloid
AUTHOR(S): Kunitomo, Junichi; Satoh, Miyoko
CORPORATE SOURCE: Fac. Pharm. Sci., Mukogawa Women's Univ., Nishinomiya, 663, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1982), 30(7), 2659-60
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The structure of the unknown yellow base from *Menispermum dauricum* DC. (Menispermaceae) was determined to be 5,6,9-trimethoxy-7H-dibenzo[de,h]quinolin-7-one (I) by spectral data and total synthesis. It was named menisporphine and the skeletal name "oxoisoaporphine" was proposed for this new type of alkaloid. The biosynthesis route of oxoisoaporphine-type alkaloids in plants is suggested.
IT 83287-04-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

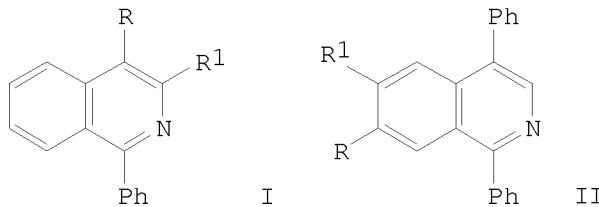
STN

RN 83287-04-1 HCAPLUS
CN Benzoic acid, 2-(6,7-dimethoxy-1-isoquinolinyl)-5-methoxy- (CA INDEX
NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS
RECORD (11 CITINGS)

L13 ANSWER 170 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:527463 HCAPLUS
DOCUMENT NUMBER: 97:127463
ORIGINAL REFERENCE NO.: 97:21153a, 21156a
TITLE: A reinvestigation of the Pictet-Gams isoquinoline synthesis. Part 2. Formation of rearranged isoquinolines: the Δ^2 -oxazoline-isoquinoline transformation
AUTHOR(S): Ardabilchi, Nasser; Fitton, Alan O.; Haidi, A. Hamid
b. A.; Thompson, J. Robin
CORPORATE SOURCE: Dep. Chem. Appl. Chem., Univ. Salford, Salford, M5
4WT, UK
SOURCE: Journal of Chemical Research, Synopses (1982
(6), 156-7
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:127463
GI

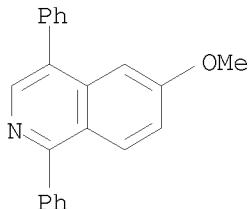


AB Cyclization of 2-substituted 2-acylamino-1-arylalkan-1-ols with P2O5 in refluxing decalin gave rearranged, i. e., 4-substituted, isoquinolines in addition to the expected 3-substituted isomers. E.g., erythro-PhCH(OH)CH(CHMe2)NHBz cyclized to give 37% of a 31:69 mixture of isoquinolines I (R = H, R1 = CHMe2; R = CHMe2, R1 = H). With

STN

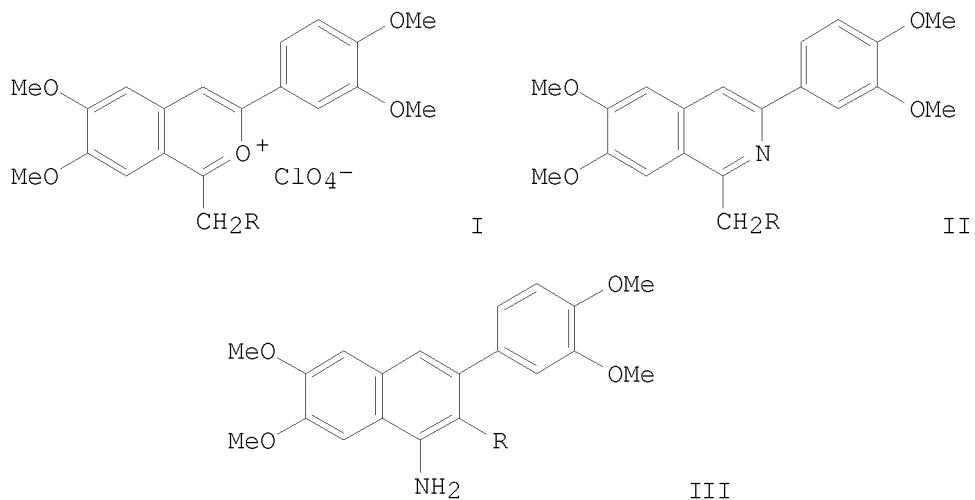
erythro-PhCH(OH)CHRNBz (R = C₆H₄OMe-3, -4), the 4-substituted isoquinolines II (R = H, R₁ = OMe; R = OMe, R₁ = H), resp., were obtained exclusively in 76 and 88% yields. The reaction involves 5-phenyl-Δ₂-oxazoline intermediates; the formation of the rearranged isoquinolines from the intermediates is discussed.

IT 82894-69-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82894-69-7 HCPLUS
CN Isoquinoline, 6-methoxy-1,4-diphenyl- (CA INDEX NAME)

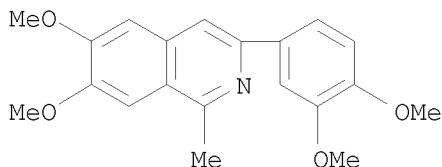


OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

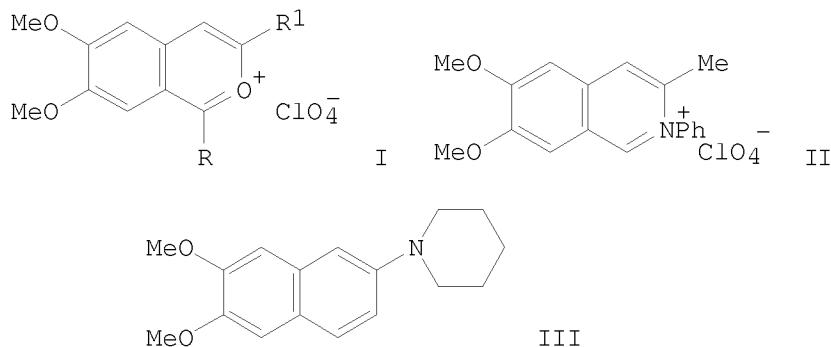
L13 ANSWER 171 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:472223 HCPLUS
DOCUMENT NUMBER: 97:72223
ORIGINAL REFERENCE NO.: 97:12085a,12088a
TITLE: Reaction of 1-alkyl-3-aryl-2-benzopyrylium salts with ammonia
AUTHOR(S): Shcherbakova, I. V.; Kuznetsov, E. V.
CORPORATE SOURCE: Nauchno-Issled. Inst. Fiz. Org. Khim., Rostov-on-Don,
344006, USSR
SOURCE: Khimiya Geterotsiklicheskih Soedinenii (1982
) , (4), 552-3
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



AB Reaction of I ($R = H, Me$) with NH₃ gave II and III, but I ($R = Ph$) gave only II.
 IT 35989-93-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 35989-93-6 HCPLUS
 CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



L13 ANSWER 172 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1982:142656 HCPLUS
 DOCUMENT NUMBER: 96:142656
 ORIGINAL REFERENCE NO.: 96:23457a, 23460a
 TITLE: 2-Benzopyrylium salts. 25. Reaction of
 2-benzopyrylium salts with some nucleophiles
 Safaryan, G. P.; Shcherbakova, I. V.; Dorofeenko, G.
 N.; Kuznetsov, E. V.
 AUTHOR(S): Rostov. Gos. Univ., Rostov, USSR
 CORPORATE SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1981
 SOURCE:), (12), 1608-11
 CODEN: KGSSAQ; ISSN: 0453-8234
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



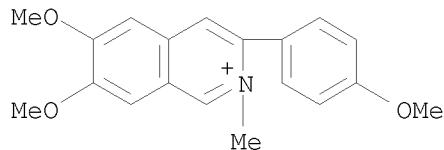
AB The structure of the products formed by reaction of I [R, R1 = H, Me (Ia); H, 4-MeOC6H4; H, 3,4-(MeO)2C6H3; Et, Me] with amines was determined not only by the nature of I, but by that of the amine. Thus, Ia and PhNH2 in EtOH refluxed 15 min gave 67% II; while with piperidine (1 h) Ia gave III.

IT 81243-43-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

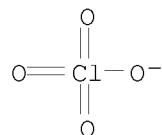
RN 81243-43-8 HCPLUS

CN Isoquinolinium, 6,7-dimethoxy-3-(4-methoxyphenyl)-2-methyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 81243-42-7
CMF C19 H20 N O3

CM 2

CRN 14797-73-0
CMF Cl O4

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD

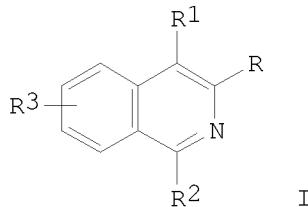
STN

(2 CITINGS)

L13 ANSWER 173 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:587098 HCAPLUS
DOCUMENT NUMBER: 95:187098
ORIGINAL REFERENCE NO.: 95:31217a,31220a
TITLE: Isoquinoline derivatives and their use for medicaments
INVENTOR(S): Bartmann, Wilhelm; Konz, Elmar; Kruse, Hansjoerg;
Geyer, Harry M.
PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.
SOURCE: U.S., 17 pp. Cont.-in-part of U.S. Ser. No. 20,411,
abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4282223	A	19810804	US 1979-76862	19790919 <--
DE 2811312	A1	19790927	DE 1978-2811312	19780316 <--
PRIORITY APPLN. INFO.:			DE 1978-2811312	A 19780316
			US 1979-20411	A2 19790314

GI



AB Antidepressant (no data) isoquinolines I (R = amino; R1 = CO₂H, cyano, CHO, CH₂OH, alkoxyethyl, aminoalkoxyethyl, acyloxyethyl, aminomethyl, carbamoyl, aminoalkoxycarbonyl, optionally substituted vinyl; R2 = optionally substituted Ph, pyridyl, thiienyl; R3 = H, halogen, OH, alkyl, alkoxy, NO₂, NH₂, OCH₂Ph, OCH₂O, OCH₂CH₂O) were prepared. Thus 20 g I (R = Cl, R1 = CHO, R2 = Ph, R3 = H) was treated with 15 g N-methylpiperazine to give 21 g I (R = N-methylpiperazino, R1 = CHO, R2 = Ph, R3 = H).

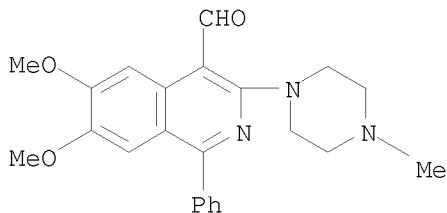
IT 72118-75-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

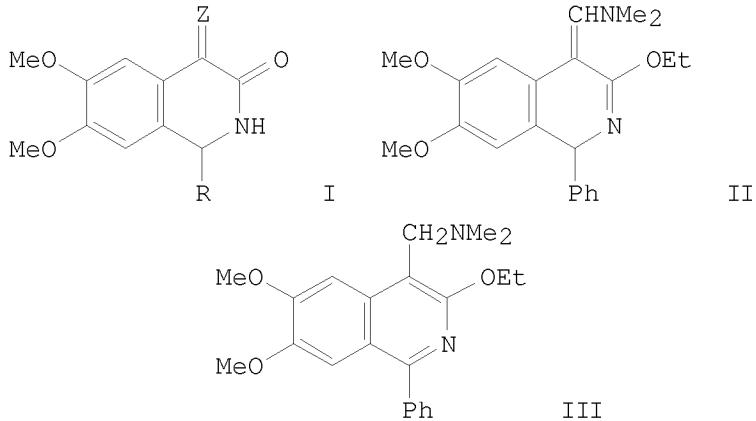
RN 72118-75-3 HCAPLUS

CN 4-Isoquinolinecarboxaldehyde, 6,7-dimethoxy-3-(4-methyl-1-piperazinyl)-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

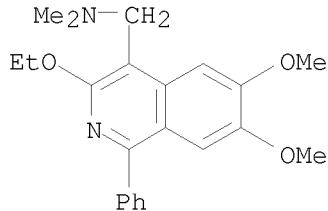
L13 ANSWER 174 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:515235 HCAPLUS
DOCUMENT NUMBER: 95:115235
ORIGINAL REFERENCE NO.: 95:19329a,19332a
TITLE: Acetals of lactams and amides of acids. 34.
Synthesis and properties of isoquinoline enamines
AUTHOR(S): Knyazeva, V. F.; Granik, V. G.; Glushkov, R. G.;
Solov'eva, N. P.; Anisimova, O. S.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow,
119021, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1981
, (4), 511-15
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 95:115235
GI



AB Condensation of isoquinolinones I ($R = H, Ph$; $Z = H_2$) with $Me_2NCH(OEt)_2$ in DMF at 100° gave I ($Z = Me_2NCH:$) which condensed with R_1NH_2 ($R_1 = PhCH_2, PhCH_2CH_2$) to give I ($Z = R_1NHCH:$). Treatment of I ($R = Ph$; $Z = Me_2NCH:$) with $Et_3O^+ \cdot BF_4^-$ and then with KOH gave ethoxyisoquinoline II, which was treated with $NaOEt$ in refluxing EtOH to give the aminomethylisoquinoline III.

STN

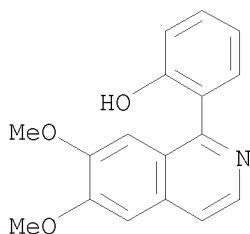
IT 78893-45-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 78893-45-5 HCAPLUS
CN 4-Isoquinolinemethanamine, 3-ethoxy-6,7-dimethoxy-N,N-dimethyl-1-phenyl-
(CA INDEX NAME)



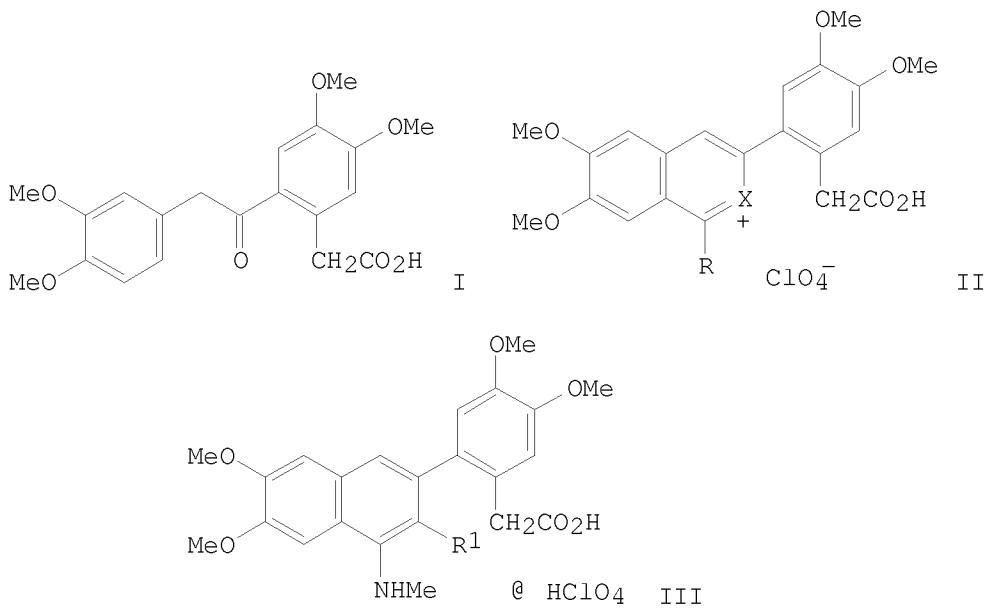
L13 ANSWER 175 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:496644 HCAPLUS
DOCUMENT NUMBER: 95:96644
ORIGINAL REFERENCE NO.: 95:16235a,16238a
TITLE: A reversible rearrangement of the trans-erythrinane ring system. IV. Studies of the reaction mechanism
AUTHOR(S): Janssen, Hans Werner; Mohr, Siegfried; Mondon, Albert
CORPORATE SOURCE: Inst. Org. Chem., Univ. Kiel, Kiel, D-2300, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1981), 114(6), 2158-85
DOCUMENT TYPE: CODEN: CHBEAM; ISSN: 0009-2940
LANGUAGE: Journal
GI German

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Acetylation of I gave II. The structure of II was confirmed by x-ray anal., and the structures of compds. emerging during the rearrangement (III, IV, and V) were confirmed by independent synthesis. Extensive labeling studies demonstrated that the rearrangement operates by a concerted 4-center mechanism with a stereospecific 1,2-shift of all groups in question.
IT 78632-08-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 78632-08-3 HCAPLUS
CN Phenol, 2-(6,7-dimethoxy-1-isoquinoliny)- (CA INDEX NAME)



L13 ANSWER 176 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:480653 HCAPLUS
DOCUMENT NUMBER: 95:80653
ORIGINAL REFERENCE NO.: 95:13635a,13638a
TITLE: 2-Benzopyrylium salts. 24. Synthesis and reactions
of salts of 3-(2-methylenecarboxyaryl)-2-benzopyrylium
with amines
AUTHOR(S): Shcherbakova, I. V.; Dorocheenko, G. N.; Kuznetsov, E.
V.
CORPORATE SOURCE: Rostov. Gos. Univ., Rostov, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1981
, (3), 313-16
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 95:80653
GI



AB Cyclocondensation the phenylacetic acid I with BuOCHCl₂ in the presence of AlCl₃ gave the benzopyrylium perchlorate II (X = O, R = H) which was

STN

aminated by MeNH₂ to give isoquinolinium perchlorate II (X = MeN, R = H). Treatment of II (X = O, R = Me, Et) with MeNH₂ gave methylaminonaphthalenes III (R₁ = H, Me).

IT 78564-48-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

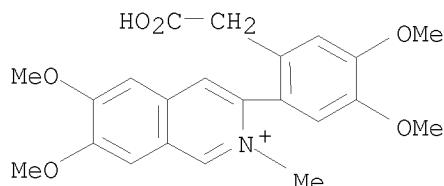
RN 78564-48-4 HCAPLUS

CN Isoquinolinium, 3-[2-(carboxymethyl)-4,5-dimethoxyphenyl]-6,7-dimethoxy-2-methyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 78564-47-3

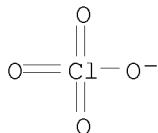
CMF C22 H24 N 06



CM 2

CRN 14797-73-0

CMF Cl O4



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 177 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1981:461957 HCAPLUS

DOCUMENT NUMBER: 95:61957

ORIGINAL REFERENCE NO.: 95:10459a,10462a

TITLE: Preparation of 1-phenyl-3-methylisoquinoline and its derivatives from oximes of 3-aryl-2-methyl-1-phenyl-2-propen-1-ones

AUTHOR(S): Zielinski, Wojciech

CORPORATE SOURCE: Inst. Org. Chem. Technol., Silesian Polytech. Univ., Gliwice, 44101, Pol.

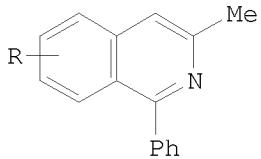
SOURCE: Polish Journal of Chemistry (1980), 54(11-12), 2209-15

CODEN: PJCHDQ; ISSN: 0137-5083

DOCUMENT TYPE: Journal

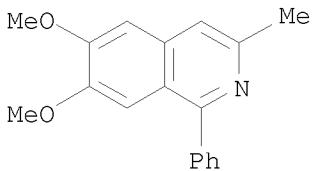
STN

LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:61957
GI



I

AB Isoquinolines I [R = H, 5-Cl, 5-MeO, 5-O2N, 6-Cl, 6-Me, 7-Cl, 7-Me, 7-MeO, 7-O2N, 6,7-(MeO)2] were obtained by treating RC6H4CHO with EtCOPh, converting RC6H4CH:CMcCOPh to their oximes, Beckmann rearrangement of the oximes with PCl5, and ring closure of the resulting imidoyl chlorides in situ.
IT 20225-88-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20225-88-1 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-3-methyl-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 178 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:424850 HCPLUS
DOCUMENT NUMBER: 95:24850
ORIGINAL REFERENCE NO.: 95:4331a,4334a
TITLE: Isoquinoline derivatives
INVENTOR(S): Bartmann, Wilhelm; Konz, Elmar
PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.
SOURCE: U.S., 8 pp. Cont.-in-part of U.S. Ser. No. 33,326,
abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4260611	A	19810407	US 1979-76204	19790917 <--
DE 2818423	A1	19791108	DE 1978-2818423	19780427 <--

STN

PRIORITY APPLN. INFO.:

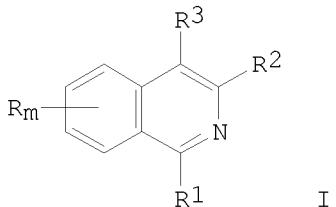
DE 1978-2818423

A 19780427

US 1979-33326

A2 19790425

GI



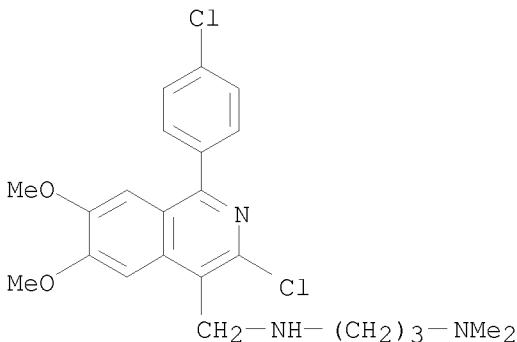
AB Isoquinolines I ($R = H$, halo, HO, alkyl, alkoxy; $R1 = Ph$, substituted phenyl; $R2 = Cl$, Br; $R3 = CO_2H$, cyano, $HOCH_2$, aminoalkyl; $m = 1, 2$), possessing antidepressant activity (no data), were prepared. Thus, KMnO₄ oxidation of 3-chloro-1-phenylisoquinoline-4-carboxaldehyde gave I ($R = H$, $R1 = Ph$, $R2 = Cl$, $R3 = CO_2H$, $m = 1$) (II). Amidation of acid chloride of II gave the N-methylpiperazide derivative

IT 78152-26-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 78152-26-8 HCPLUS

CN 1,3-Propanediamine, N3-[3-chloro-1-(4-chlorophenyl)-6,7-dimethoxy-4-isooquinolinyl]methyl]-N1,N1-dimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 179 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1981:173953 HCPLUS

DOCUMENT NUMBER: 94:173953

ORIGINAL REFERENCE NO.: 94:28419a,28422a

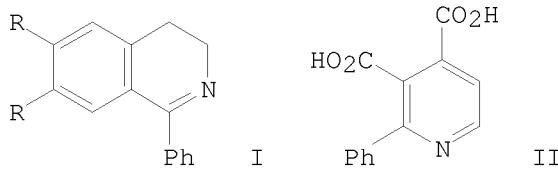
TITLE: Vanadic oxidation of 1-phenyl 3,4 dihydro isoquinolines. Effect of acidity on the reaction mechanism

AUTHOR(S): Tsitini-Tsamis, M.; Chaigneau, M.; Likforman, J.; Hamon, M.

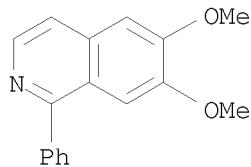
CORPORATE SOURCE: Lab. Chim. Anal., Fac. Sci. Pharm. Biol.,

STN

SOURCE: Chatenay-Malabry, 92290, Fr.
Analusis (1980), 8(9), 428-34
CODEN: ANLSCY; ISSN: 0365-4877
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



AB The oxidation of I ($R = H$) by V2O5 in H₂SO₄ gave o-BzC₆H₄CO₂H. Similarly, oxidation of I ($R = OMe$) gave 4,5,2-(MeO)2BzC₆H₂CO₂H in 2.5 M H₂SO₄ and II and HCHO in 5 M H₂SO₄. The ¹³C NMR and mass spectra of II are discussed. The time dependence and mechanism of these reactions are also discussed.
IT 4029-09-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 4029-09-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)

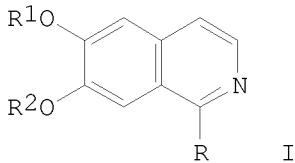


L13 ANSWER 180 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1980:610276 HCPLUS
DOCUMENT NUMBER: 93:210276
ORIGINAL REFERENCE NO.: 93:33465a,33468a
TITLE: Hair conditioner with anti-flaking activity
INVENTOR(S): Moeller, Hinrich; Thimm, Hans Joachim
PATENT ASSIGNEE(S): Henkel K.-G.a.A., Fed. Rep. Ger.
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

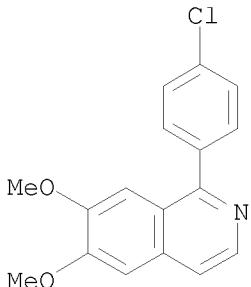
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2851283	A1	19800612	DE 1978-2851283	19781127 <--
EP 11821	A2	19800611	EP 1979-104639	19791122 <--
EP 11821	A3	19810114		

STN

R: BE, CH, DE, FR, GB, IT, NL, SE
AT 7907485 A 19810415 AT 1979-7485 19791126 <--
AT 364713 B 19811110
PRIORITY APPLN. INFO.: DE 1978-2851283 A 19781127
GI



AB Isoquinoline derivs. I (R = alkyl, or substituted Ph or benzyl, R1 and R2 = Me or Et) show antidandruff (antiflaking) activity and are formulated in hair preps. In a test on guinea pigs papaverine [58-74-2] showed inhibition of skin thickening and antidandruff activity. Hair preps. and shampoos were prepared containing I such as I (R = PhCH₂, R1 = R2 = Me) [23818-73-7], I (R = Et, R1 = R2 = Me) [18033-30-2], or I (R = 4-ClC₆H₄, R1 = R2 = Me) [75448-45-2].
IT 75448-45-2
RL: BIOL (Biological study)
(antidandruff hair preps. containing)
RN 75448-45-2 HCPLUS
CN Isoquinoline, 1-(4-chlorophenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 181 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1980:603556 HCPLUS
DOCUMENT NUMBER: 93:203556
ORIGINAL REFERENCE NO.: 93:32465a,32468a
TITLE: 2,3-Benzodiazepines: 2-aminoisoquinolinones from ring contraction of 1-oxo-2,3-benzodiazepines
AUTHOR(S): Flammang, Michel; Wermuth, Camille Georges
CORPORATE SOURCE: Lab. Chim. Org. Therap., CNRS, Strasbourg, 67048, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1980), 290(18), 361-3

STN

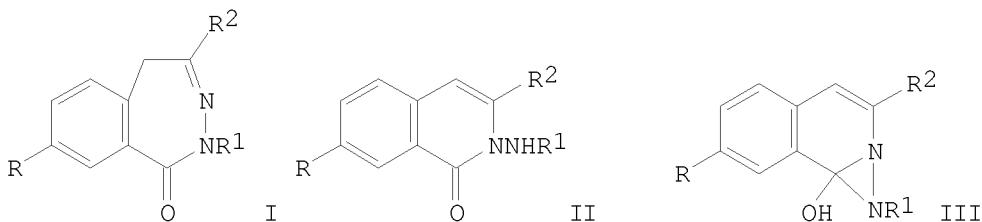
DOCUMENT TYPE:
LANGUAGE:
OTHER SOURCE(S):
GI

CODEN: CHDCAQ; ISSN: 0567-6541

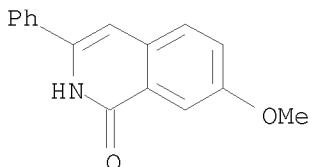
Journal

French

CASREACT 93:203556



AB Heating I ($R = H, OMe$; $R1 = H, Me$, morpholinoethyl; $R2 = \text{aryl}$) in acid gives the corresponding II in a ring contraction via III. This reaction depends mainly on the nature of $R1$. The best yields are obtained with $R1$ is H .
IT 62265-91-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 62265-91-2 HCPLUS
CN 1(2H)-Isoquinolinone, 7-methoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 182 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1980:560962 HCPLUS
DOCUMENT NUMBER: 93:160962
ORIGINAL REFERENCE NO.: 93:25489a,25492a
TITLE: Structural determinants responsible for the biological activity of (-)-emetine, (-)-cryptopleurine, and (-)-tylocrebrine: structure-activity relationship among related compounds
AUTHOR(S): Gupta, Radhey S.; Krepinsky, Jiri J.; Siminovitch, Louis
CORPORATE SOURCE: Dep. Med. Biochem., McMaster Univ., Hamilton, ON, L8N 3Z5, Can.
SOURCE: Molecular Pharmacology (1980), 18(1), 136-43
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The structural basis for the cross-resistance and the common site of the protein formation inhibitory action of the benzoisoquinoline alkaloids, (-)-emetine (I) [483-18-1], tubulosine [2632-29-3], (-)-cephaeline [483-17-0], and (-)-dehydroemetine [4914-30-1], and of the phenanthroquinolizidine-type alkaloids, (-)-cryptopleurine (II) [482-22-4], and the phenanthroindolizidine type, (-)-tylocrebrine (III) [61302-92-9], was investigated by examining the cross-resistance of emetine-resistant mutants of Chinese hamster ovary cells to a large number of related compds. These compds. possess common structural determinants which are responsible for their biol. activity. The requirement for biol. activity is a planar mol. with 2 aromatic rings (rendered slightly electron richer, i.e. electroneg. by methoxyl or hydroxyl groups) and the presence of a nucleophilic element such as N at a certain distance from the aromatic rings. The distance between the 2 aromatic rings, the angle between the N atom and the rings, and the electroneg. character of the rings and planarity of the structure are critical features in determining the biol. activity.

The absolute configurations of (-)-cryptopleurine and (-)-tylocrebrine are proposed.

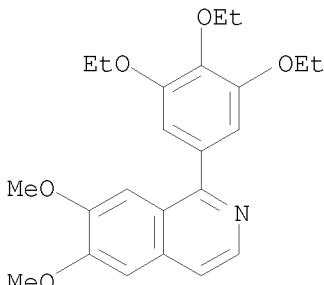
IT 549-68-8

RL: BIOL (Biological study)

(protein formation inhibition by, structure in relation to)

RN 549-68-8 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)

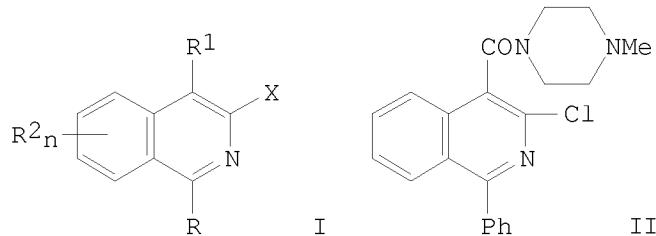


OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

L13 ANSWER 183 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1980:110874 HCAPLUS
 DOCUMENT NUMBER: 92:110874
 ORIGINAL REFERENCE NO.: 92:18093a,18096a
 TITLE: Isoquinoline derivatives
 INVENTOR(S): Bartmann, Wilhelm; Konz, Elmar
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 26 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

STN

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2818423	A1	19791108	DE 1978-2818423	19780427 <--
EP 5231	A2	19791114	EP 1979-101232	19790424 <--
EP 5231	A3	19800903		
EP 5231	B1	19821215		
R: CH, DE, FR, GB				
JP 54154773	A	19791206	JP 1979-50942	19790426 <--
US 4260611	A	19810407	US 1979-76204	19790917 <--
PRIORITY APPLN. INFO.:			DE 1978-2818423	19780427
			US 1979-33326	A2 19790425
OTHER SOURCE(S):	MARPAT	92:110874		
GI				



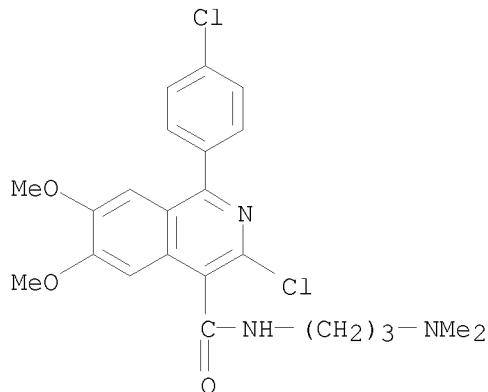
AB A wide range of I (X = Cl or Br, R = aryl, R1 = CO2H, cyano, substituted amino, etc., n = 1 or 2, R2 = H, halogen, OH, etc.) were prepared as antiarrhythmics, antipyretics, and tranquilizers (no data). Thus, oxidation of 3-chloro-1-phenyl-4-isoquinolinecarboxaldehyde, with KMnO4 gave the acid, which was converted into the acid chloride with SOC12 and treated with N-methylpiperazine to give II.

IT 72736-28-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and borohydride reduction of)

RN 72736-28-8 HCPLUS

CN 4-Isoquinolinecarboxamide, 3-chloro-1-(4-chlorophenyl)-N-[3-(dimethylamino)propyl]-6,7-dimethoxy- (CA INDEX NAME)

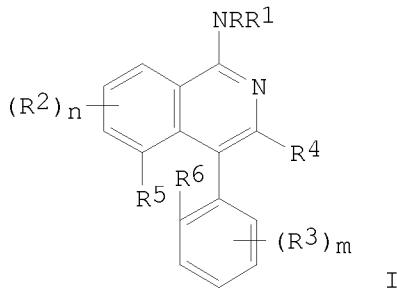


STN

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 184 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1980:22393 HCAPLUS
DOCUMENT NUMBER: 92:22393
ORIGINAL REFERENCE NO.: 92:3809a,3812a
TITLE: 1-Amino-4-phenylisoquinoline derivatives
INVENTOR(S): Simmonds, Robin George
PATENT ASSIGNEE(S): Aspro-Nicholas Ltd., UK
SOURCE: Brit., 16 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	-----	-----	-----	-----
GB 1545767	A	19790516	GB 1975-31144	19760630 <--
PRIORITY APPLN. INFO.:			GB 1975-31144	19760630
GI				



AB The preparation is described of title compds. I (R, R1 = H, C1-12 alkyl; RNR1 = piperazinyl optionally substituted by C1-12 alkyl or hydroxyalkyl; n = 0 - 3; m = 0 - 4; R2,R3 = C1-12 alkyl optionally substituted by ≥1 halo, C1-12 alkoxy, halo; R4 = H, C1-12 alkyl; R5,R6 = H or C1-12 alkyl, alkylthio, alkoxy; R5R6 = bond, O, S, C1-3 alkylene optionally containing ≥1 O or S), which show antiinflammatory (especially antirheumatic) and/or central nervous system activity. Thus, 3-dimethylamino-7,8-dihydrobenzo[1,2]cyclohepta[3.4.5-de]isoquinoline hydrogen maleate was prepared from dibenzo[ad]suberone by sequential treatment with NaH/Me3S+ I-, BF3.Me2O/CH2Cl2, and H2NCO2Et/H2SO4 followed by heating (256°, 1 h), refluxing with POCl3, and Me2NH/EtOH treatment. The yields of the 6 steps were 96, 98, 100, 89, 99, and 75.6%, resp. Compns. containing I are described.

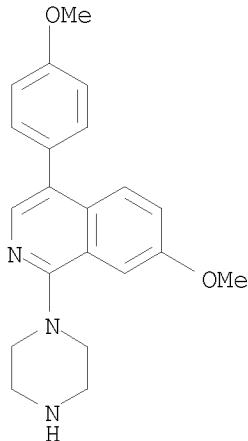
IT 72240-34-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(inflammation inhibitor, preparation of)

RN 72240-34-7 HCAPLUS

CN Isoquinoline, 7-methoxy-4-(4-methoxyphenyl)-1-(1-piperazinyl)- (CA INDEX NAME)

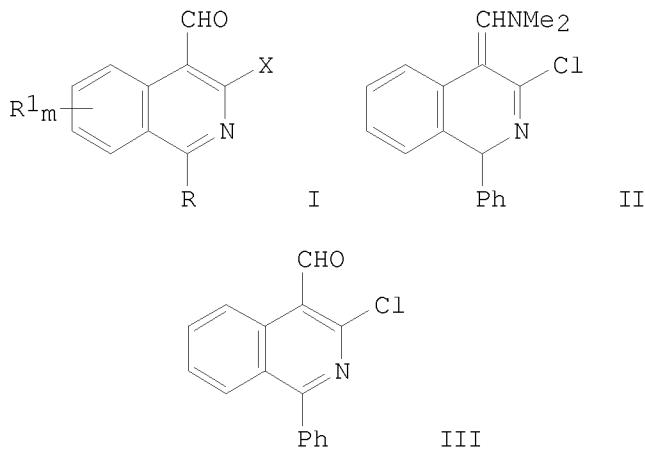
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OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(14 CITINGS)

L13 ANSWER 185 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1980:6431 HCAPLUS
DOCUMENT NUMBER: 92:6431
ORIGINAL REFERENCE NO.: 92:1207a,1210a
TITLE: Isoquinoline aldehydes
INVENTOR(S): Bartmann, Wilhelm; Konz, Elmar; Kruse, Hansjoerg
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2811361	A1	19790927	DE 1978-2811361	19780316 <--
EP 4322	A1	19791003	EP 1979-100712	19790309 <--
EP 4322	B1	19801029		
R: CH, DE, FR, US 4260763	GB A	19810407	US 1979-20410	19790314 <--
JP 54130582	A	19791009	JP 1979-31651	19790316 <--
PRIORITY APPLN. INFO.:			DE 1978-2811361	19780316
OTHER SOURCE(S): GI	MARPAT	92:6431		



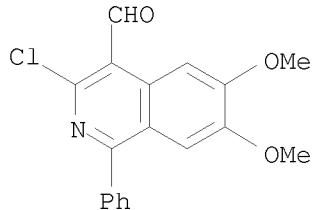
AB I ($X = \text{Br or Cl}$; $R = \text{aryl, pyridyl, or thienyl}$; $R^1 = \text{H or, e.g., halogen, alkyl, or alkoxy}$; $m = 1 \text{ or } 2$) were prepared Thus, 56 g 1,4-dihydro-1-phenyl-3(2H)-isoquinolinone were added at 20–35° to 73 mL DMF and 146 g POCl_3 in 400 mL THF at 20–35° to give 71% II, which was oxidized with KMnO_4 to give 90% III.

IT 72179-16-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 72179-16-9 HCAPLUS

CN 4-Isoquinolinecarboxaldehyde, 3-chloro-6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 186 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1980:6430 HCAPLUS

DOCUMENT NUMBER: 92:6430

ORIGINAL REFERENCE NO.: 92:1207a,1210a

TITLE: Isoquinoline derivatives

INVENTOR(S): Bartmann, Wilhelm; Konz, Elmar; Kruse, Hansjoerg;
Geyer, Harry Maurice

PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 55 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

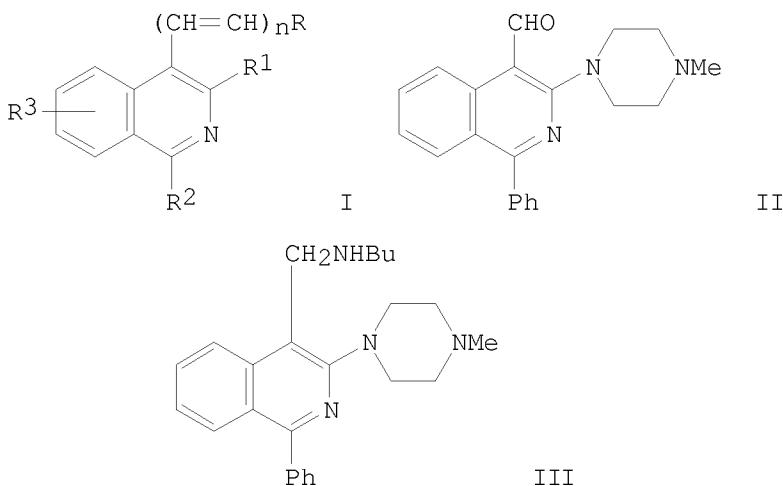
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

STN

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2811312	A1	19790927	DE 1978-2811312	19780316 <--
EP 4332	A1	19791003	EP 1979-100737	19790312 <--
EP 4332	B1	19810826		
R: CH, DE, FR, GB US 4282223	A	19810804	US 1979-76862 DE 1978-2811312 US 1979-20411	19790919 <-- 19780316 A2 19790314
PRIORITY APPLN. INFO.:				
OTHER SOURCE(S):	MARPAT	92:6430		
GI				



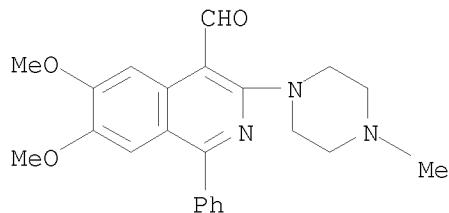
AB A series of .apprx.100 I, in most of which n = 0 or 1, R = CHO, CH₂OH, or substituted amino or amide, R₁ = substituted amino, R₂ = aryl, R₃ = H, 6-Cl, or 6,7-(methylenedioxy) were prepared as sedatives and muscle relaxants (no data). Thus 3-chloro-1-phenyl-4-isoquinolinecarboxaldehyde was treated with 1-methylpiperazine to give II. Also prepared was, e.g., III.

IT 72118-75-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and borohydride reduction of)

RN 72118-75-3 HCPLUS

CN 4-Isoquinolinecarboxaldehyde, 6,7-dimethoxy-3-(4-methyl-1-piperazinyl)-1-phenyl- (CA INDEX NAME)

STN

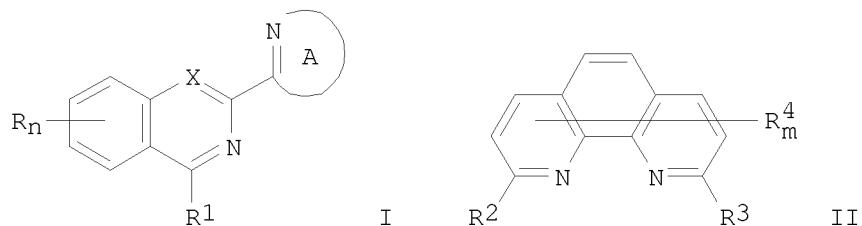


OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 187 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:439514 HCAPLUS
DOCUMENT NUMBER: 91:39514
ORIGINAL REFERENCE NO.: 91:6449a,6452a
TITLE: Copper complexes of phenanthroline, isoquinoline, and quinazoline derivatives useful in combatting mycoplasma infections
INVENTOR(S): Nauta, W. T.
PATENT ASSIGNEE(S): Gist-Brocades N. V., Neth.
SOURCE: Ger. Offen., 62 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2826526	A1	19790104	DE 1978-2826526	19780616 <--
NL 7713938	A	19790619	NL 1977-13938	19771215 <--
GB 2002746	A	19790228	GB 1978-27117	19780616 <--
DK 7802750	A	19781218	DK 1978-2750	19780619 <--
SE 7807001	A	19781218	SE 1978-7001	19780619 <--
BE 868249	A1	19781219	BE 1978-188676	19780619 <--
NL 7806573	A	19781219	NL 1978-6573	19780619 <--
FR 2401155	A1	19790323	FR 1978-18282	19780619 <--
US 4269834	A	19810526	US 1978-916541	19780619 <--
CA 1102329	A1	19810602	CA 1978-305746	19780619 <--
FR 2422659	A1	19791109	FR 1979-6395	19790313 <--
PRIORITY APPLN. INFO.:			GB 1977-25539	A 19770617
			NL 1977-13938	A 19771215

OTHER SOURCE(S): MARPAT 91:39514
GI



STN

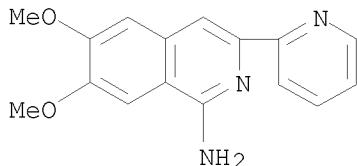
AB Cu complexes of I [R = H, alkyl, halogen; R1 = H, halogen, Ph, (alkyl-substituted) NH₂; n = 1-4; A = (substituted) pyridyl or 2-imidazolyl; X = N, alkylidene] or II (R₂ = R₃ = H, halogen, alkyl, alkoxy, NH₂; R₄ = H, alkyl, halogen; m = 1-6) were prepared for use as antimycoplastic agents (test data tabulated). Thus, 2-MeC₆H₄CN was added to K in liquid NH₃, followed by the addition of 1-methyl-2-cyano-1H-imidazole to give I (R_n = H, R₁ = NH₂, X = CH, A = 1-methyl-2-imidazolyl), which reacted with CuNO₂ to give the Cu(I) complex.

IT 69767-44-8DP, copper complex

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and mycoplasma inhibition by)

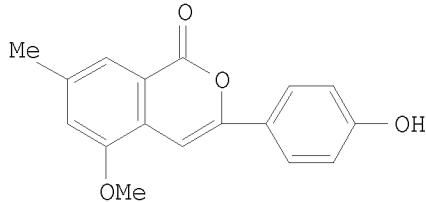
RN 69767-44-8 HCPLUS

CN 1-Isoquinolinamine, 6,7-dimethoxy-3-(2-pyridinyl)- (CA INDEX NAME)

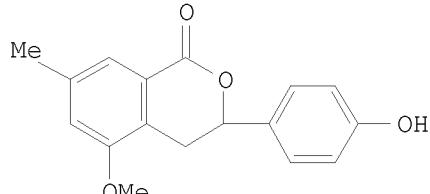


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

L13 ANSWER 188 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:405071 HCPLUS
DOCUMENT NUMBER: 91:5071
ORIGINAL REFERENCE NO.: 91:950h,951a
TITLE: Synthesis of some
3-aryl-5-methoxy-7-methylisocoumarins
AUTHOR(S): Sarkhel, B. K.; Srivastava, Jagadish N.
CORPORATE SOURCE: Dep. Chem., Bhagalpur Univ., Bhagalpur, 812007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic
Chemistry Including Medicinal Chemistry (1978
, 16B(11), 1034-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 91:5071
GI



I



II

AB Phenol, anisole, o-cresol, m-cresol and p-cresol were condensed with

6-methoxy-4-methylhomophthalic acid in the presence of polyphosphoric acid to give 3-(4-hydroxyphenyl) (I), 3-(4-methoxyphenyl), 3-(4-hydroxy-3-methylphenyl), 3-(2-hydroxy-4-methylphenyl), and 3-(2-hydroxy-5-methylphenyl)-5-methoxy-7-methylisocoumarins. On treatment with aqueous NaOH, the coumarins yield the resp.

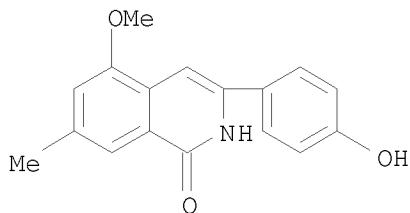
α -(2-carboxy-4-methyl-6-methoxyphenyl)acetophenones, which with NaBH₄ reduction gave the corresponding dihydroisocoumarins, e.g. II, which were transformed into the parent isocoumarins by treatment with N-bromosuccinimide followed by refluxing in pyridine. The isocoumarins were characterized as 1(2H)-isoquinolones.

IT 70351-69-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 70351-69-8 HCPLUS

CN 1(2H)-Isoquinolinone, 3-(4-hydroxyphenyl)-5-methoxy-7-methyl- (CA INDEX NAME)



L13 ANSWER 189 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1979:121376 HCPLUS

DOCUMENT NUMBER: 90:121376

ORIGINAL REFERENCE NO.: 90:19211a, 19214a

TITLE: Synthesis of 3-arylisquinolines by thermolysis of 3-aryl-1,2-dihydroisoquinolin-4(3H)-one salts

AUTHOR(S): Livingstone, David A.; Waigh, Roger D.

CORPORATE SOURCE: Dep. Pharm. Chem., Univ. Strathclyde, Glasgow, UK

SOURCE: Journal of the Chemical Society, Chemical

Communications (1978), (23), 1026-7

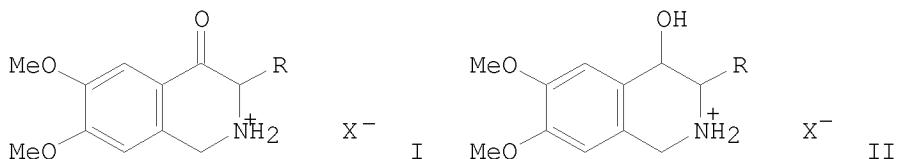
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 90:121376

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AB Heating dihydroquinolinone salts I [X = HSO₄, R = Ph, 3,4-C₁₂C₆H₃; X = Cl,

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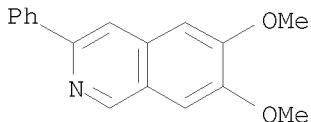
R = 4-pyridyl, 3,4-(MeO)2C6H3] in DMF gave mixts. of the corresponding 3-arylisoquinolines (23-64%) and 3-aryl-4-hydroxyisoquinolines (14-44%). An intermol. mechanism is proposed in which tetrahydroisoquinolines II are regenerated in a cyclic process.

IT 24285-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24285-10-7 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-3-phenyl- (CA INDEX NAME)



L13 ANSWER 190 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1978:145964 HCPLUS

DOCUMENT NUMBER: 88:145964

ORIGINAL REFERENCE NO.: 88:22882h,22883a

TITLE: Correlation between the hydrolysis constants and spasmolytic activities of some isoquinolines

AUTHOR(S): Simon, L.; Poreszsz, J.; Gibiszer, P. Katalin; Talpas, S. G.

CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Med. Sch. Szeged, Szeged, Hung.

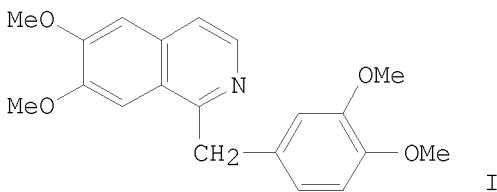
SOURCE: Pharmazie (1977), 32(11), 720-1

CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

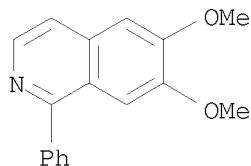


AB The spasmolytic activities of the isoquinoline alkaloids papaverine-HCl (I-HCl) [61-25-6], ethaverine-HCl [985-13-7], drotaverine-HCl [985-12-6], S-8 (1-phenyl-6,7-dimethoxyisoquinoline-HCl) [63768-18-3], S-7 (1-phenyl-6,7-dimethoxy-3,4-dihydroisoquinoline-HCl) [10133-76-3], and S-23 (1-phenyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline-HCl) [63768-20-7] against BaCl2-induced contractions of the isolated guinea pig ileum were dependent upon the hydrolysis consts. of the alkaloids; the greater the hydrolysis constant, the stronger was the spasmolytic activity. The spasmolytic activities of

STN

these compds. apparently were due to the base form of the alkaloids. Acidification reduced the quantity of free base and decreased the spasmolytic activities.

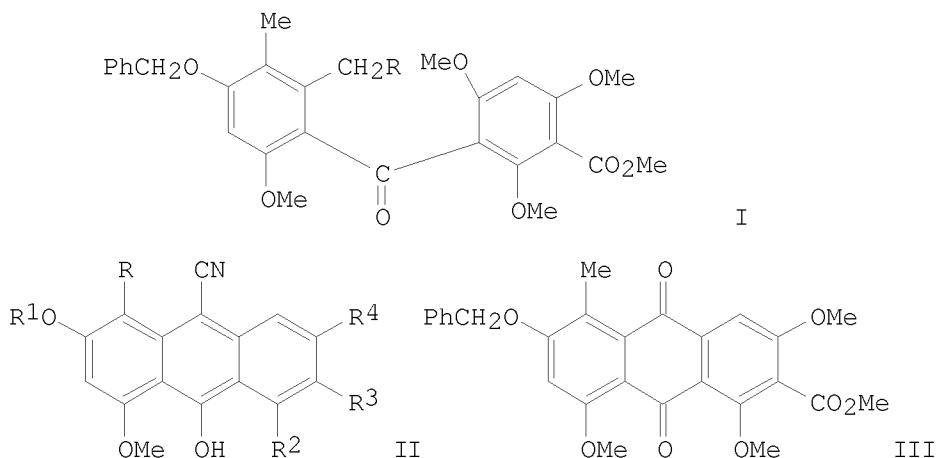
IT 63768-18-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(spasmolytic activity of, hydrolysis constant in relation to)
RN 63768-18-3 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 191 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1978:136350 HCPLUS
DOCUMENT NUMBER: 88:136350
ORIGINAL REFERENCE NO.: 88:21427a,21430a
TITLE: Tetracycline studies. Part 5. New syntheses of anthracenes and anthraquinones through benzophenone carbanions
AUTHOR(S): Broadhurst, Michael J.; Hassall, Cedric H.; Thomas, Gareth J.
CORPORATE SOURCE: Roche Prod. Ltd., Welwyn Garden City, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1977), (22), 2502-12
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



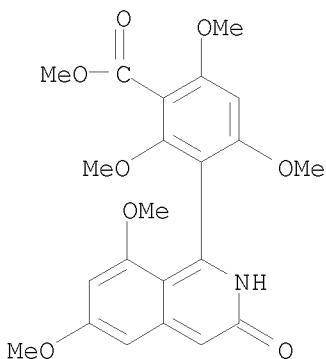
AB The title syntheses are of wide applicability and gave good yields of products. E.g., the benzophenone I (R = CN) with Me₃COK in DMF at 90° for 1 h gave 95% anthrhol II (R = Me, R₁ = PhCH₂, R₂ = R₄ = OMe, R₃ = CO₂Me) which with H₂O₂ and NaOH gave 96% anthraquinone III. I (R = CO₂Me) with Me₃COK in DMF followed by H₂O₂-NaOH treatment gave 41% III. Regiospecificity of cyclization was achieved by preferential displacement of Cl-. E.g., 2-(2,4-dichlorobenzoyl)-3,5-dimethoxyphenylacetonitrile with Me₃COK in DMF gave 46% II (R = R₂ = R₃ = H, R₁ = Me, R₄ = Cl). In some circumstances 2-cyanomethylbenzophenones with (F₃CCO)₂O gave isoquinolin-3-one derivs.

IT 65977-07-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 65977-07-3 HCPLUS

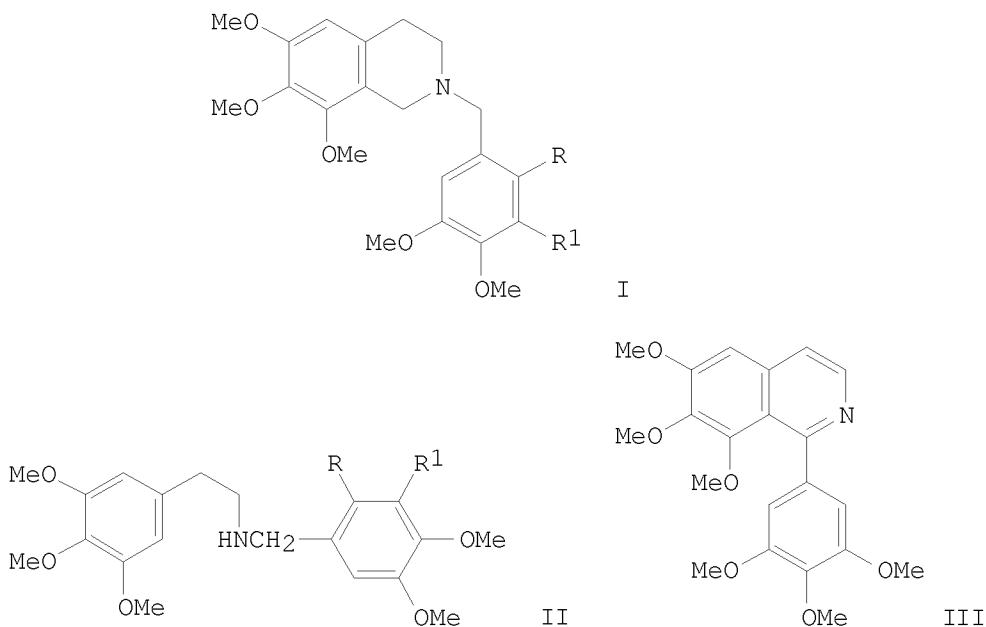
CN Benzoic acid, 3-(2,3-dihydro-6,8-dimethoxy-3-oxo-1-isoquinolinyl)-2,4,6-trimethoxy-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

L13 ANSWER 192 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1978:121486 HCAPLUS
 DOCUMENT NUMBER: 88:121486
 ORIGINAL REFERENCE NO.: 88:19081a,19084a
 TITLE: Polymethoxylated isoquinolines as potential antimitotic agents
 AUTHOR(S): Iorio, Maria; Brossi, Arnold; Chignell, Colin F.
 CORPORATE SOURCE: Lab. Chem., Natl. Inst. Arthritis, Metab. Dig. Dis., Bethesda, MD, USA
 SOURCE: Heterocycles (1978), 9(1), 1-6
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

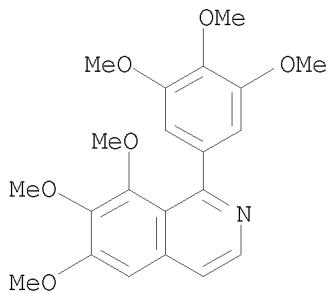


AB The sendaverine derivs. I ($R = \text{MeO}$, $R1 = \text{H}$; $R = \text{H}$, $R1 = \text{MeO}$) were prepared by condensation of mescaline with 2,4,5-(MeO)3C6H2CHO and 3,4,5-(MeO)3C6H2CHO and reduction of the Schiff bases to give II, which were cyclized. The cryptostyline derivative III was prepared by cyclization of 3,4,5-(MeO)3C6H2CONHCH2CH2C6H2(OMe)3-3,4,5 followed by reduction and dehydrogenation. Using colchicine as a standard none of the compds. showed any binding affinity to the rat brain microtubule protein.

IT 65967-40-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

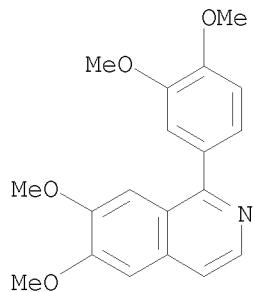
RN 65967-40-0 HCAPLUS

CN Isoquinoline, 6,7,8-trimethoxy-1-(3,4,5-trimethoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

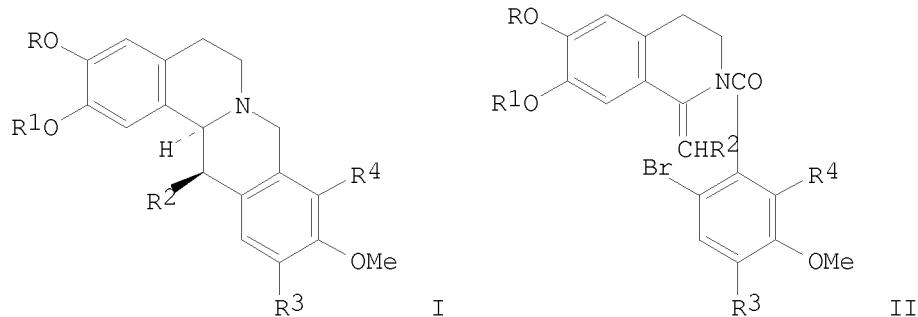
L13 ANSWER 193 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1977:561444 HCPLUS
 DOCUMENT NUMBER: 87:161444
 ORIGINAL REFERENCE NO.: 87:25435a,25438a
 TITLE: Inhibition of catechol O-methyltransferase and transfer RNA methyltransferases by coralyne, nitidine, and related compounds
 AUTHOR(S): Lee, John W.; MacFarlane, John O.; Zee-Cheng, Robert K. Y.; Cheng, C. C.
 CORPORATE SOURCE: Midwest Res. Inst., Kansas City, MO, USA
 SOURCE: Journal of Pharmaceutical Sciences (1977), 66(7), 986-9
 CODEN: JPMSAE; ISSN: 0022-3549
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Inhibitory activity against both catechol O-methyltransferase [9012-25-3] and transfer RNA methyltransferase [9014-53-3] was observed among the antileukemic alkaloids coralyne acetosulfate [50432-85-4], nitidine methosulfate [41349-35-3], and related synthetic alkoxy analogs. Inhibition of both classes of enzymes had a similar profile. The role of water soluble of these compds. with regard to their enzyme inhibitory activity was noted.
 IT 36455-58-0
 RL: BIOL (Biological study)
 (catechol O-methyltransferase and tRNA methyl transferase inhibition by)
 RN 36455-58-0 HCPLUS
 CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-, hydrochloride (1:1)
 (CA INDEX NAME)



● HCl

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 194 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1977:517978 HCAPLUS
DOCUMENT NUMBER: 87:117978
ORIGINAL REFERENCE NO.: 87:18745a,18748a
TITLE: Studies on the synthesis of heterocyclic compounds.
Part 698. An alternative protoberberine synthesis;
total synthesis of (\pm)-xylopinine,
(\pm)-schefferine, (\pm)-nandinine,
(\pm)-corydaline, and (\pm)-thalictropicavine
AUTHOR(S): Kametani, Tetsuji; Sugai, Toshiji; Shoji, Yohko;
Honda, Toshio; Satoh, Fumio; Fukumoto, Keiichiro
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1972-1999) (1977), (10), 1151-5
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



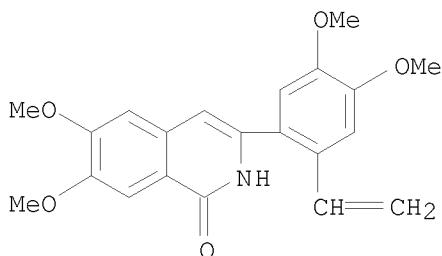
AB (\pm)-Xylopinine (I; R = R₁ = Me, R₂ = R₄ = H, R₃ = OMe),
(\pm)-schefferine (I; R = R₁ = Me, R₂ = R₃ = H, R₄ = OH), and

(\pm)-nandinine (I; RR1 = CH₂, R2 = R3 = H, R4 = OH) were prepared from the corresponding bromo enamides II by photochem. cyclization followed by reduction (\pm)-Corydaline (I; R = R1 = R2 = Me, R3 = H, R4 = OMe) and (\pm)-thalicticavine (I; RR1 = CH₂, R2 = Me, R3 = H, R4 = OMe) were prepared from the corresponding bromo enamides II by sequential photochem. cyclization, reduction, and methylation. (\pm)-Xylopinine was also prepared, together with the corresponding styrenederiv., from the corresponding II under benzyne reaction conditions.

IT 60315-12-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)

RN 60315-12-0 HCPLUS

CN 1(2H)-Isoquinolinone, 3-(2-ethenyl-4,5-dimethoxyphenyl)-6,7-dimethoxy-
(CA INDEX NAME)

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

L13 ANSWER 195 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1977:511537 HCPLUS
DOCUMENT NUMBER: 87:111537
ORIGINAL REFERENCE NO.: 87:17629a,17632a
TITLE: Physicochemical properties and membrane action of spasmolytically active isoquinoline and 1,2,3,4-tetrahydroisoquinoline derivatives
AUTHOR(S): Simon, L.; Porszasz, J.; Gibiszerkatalin, P.; Talpas, S. G.
CORPORATE SOURCE: Pharm.-Chem. Inst., Med. Univ. Szeged, Szeged, Hung.
SOURCE: Pharmazie (1977), 32(4), 235-9
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Papaverine [58-74-2], ethaverine [486-47-5], drotaverine [14009-24-6], 1-phenyl-6,7-dimethoxyisoquinoline-HCl [63768-18-3], 6,7-dimethoxyisoquinoline-HCl [63768-19-4], and isoquinoline-HCl [21364-46-5] at pH 7.6 increased the transmembrane potential and compensation current in isolated frog skin. A pH 5.9 they had an opposite effect. The 1,2,3,4-tetrahydroisoquinoline derivs., 1,2,3,4-tetrahydroisoquinoline-HCl [14099-81-1], 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline-HCl [2328-12-3], 1-phenyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline-HCl [63768-20-7], 1-benzyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline [3423-37-8], 1-p-chlorophenyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline [55507-15-8], 1-p-carbethoxyphenyl-6,7-dimethoxy-,1,2,3,4-

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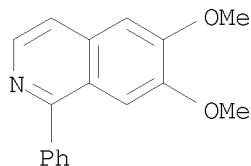
tetrahydroisoquinoline-HCl [52947-23-6],
1-p-nitrophenyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline-HCl
[4728-52-3], decreased transmembrane potential at pH 7.6. The hydrophilic
and basic properties of the isoquinoline derivs. were presented.

IT 63768-18-3

RL: BIOL (Biological study)
(skin membrane potential response to)

RN 63768-18-3 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-phenyl-, hydrochloride (1:1) (CA INDEX
NAME)



● HCl

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 196 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1977:439227 HCPLUS

DOCUMENT NUMBER: 87:39227

ORIGINAL REFERENCE NO.: 87:6182h,6183a

TITLE: 2-Benzopyrylium salts. XX. Synthesis of some
deoxybenzoins and 2-benzopyrylium salts

AUTHOR(S): Kuznetsov, E. V.; Shcherbakova, I. V.; Ushakov, V. I.;
Dorofeenko, G. N.

CORPORATE SOURCE: Nauchno-Issled. Inst. Fiz. Org. Khim., Rostov-on-Don,
USSR

SOURCE: Zhurnal Organicheskoi Khimii (1977), 13(3),
631-4

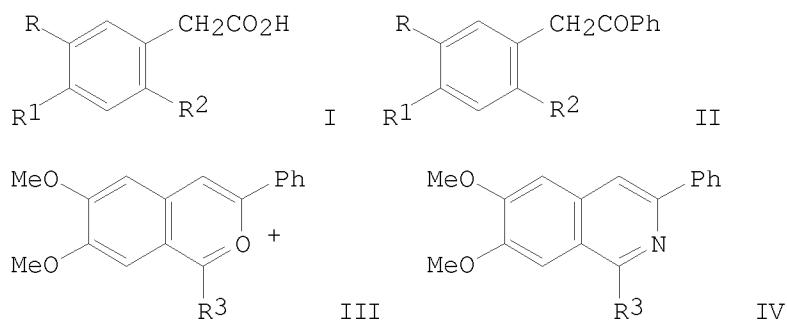
CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 87:39227

GI



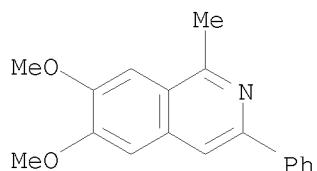
AB Reaction of acids I ($R = R_1 = R_2 = H$; $R = R_1 = \text{MeO}$, $R_2 = \text{Br}$, H) with Bz_2O in the presence of NaOAc gave 46–70% II. Treatment of II ($R = R_1 = \text{MeO}$, $R_2 = \text{Br}$) with R_3COX ($\text{R}_3 = \text{Me}$, Et , Ph , PhCH_2 , $X = \text{R}_3\text{CO}_2$, Cl , OH) gave 65–90% III, which when treated with NH_4OAc in HOAc gave 67–70% IV ($\text{R}_3 = \text{Me}$, Ph).

IT 52947-33-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

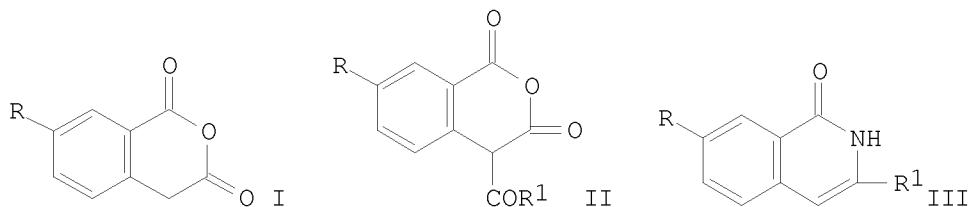
RN 52947-33-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-methyl-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 197 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1977:121133 HCPLUS
DOCUMENT NUMBER: 86:121133
ORIGINAL REFERENCE NO.: 86:19123a,19126a
TITLE: A new method for the synthesis of 3-phenylisoquinolones
AUTHOR(S): Modi, A. R.; Usgaonkar, R. N.
CORPORATE SOURCE: Org. Chem. Dep., Inst. Sci., Bombay, India
SOURCE: Current Science (1976), 45(23), 832-3
CODEN: CUSCAM; ISSN: 0011-3891
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



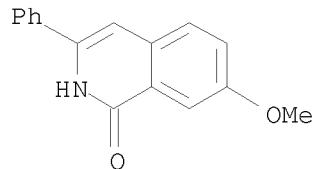
AB Acylation of the anhydrides I ($R = H, OMe$) with R_1COCl ($R_1 = Ph, Me$) gave II (not isolated) which with NH_3 gave the isoquinolones III.

IT 62265-91-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 62265-91-2 HCPLUS

CN 1(2H)-Isoquinolinone, 7-methoxy-3-phenyl- (CA INDEX NAME)



L13 ANSWER 198 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1976:508835 HCPLUS

DOCUMENT NUMBER: 85:108835

ORIGINAL REFERENCE NO.: 85:17477a, 17480a

TITLE: Alternative synthesis of protoberberine alkaloid
 (\pm) -xylopinine

AUTHOR(S): Kametani, Tetsuji; Honda, Toshio; Sugai, Toshiji;
Fukumoto, Keiichiro

CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, Japan

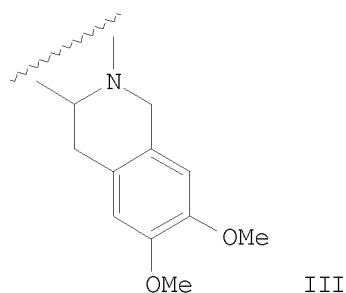
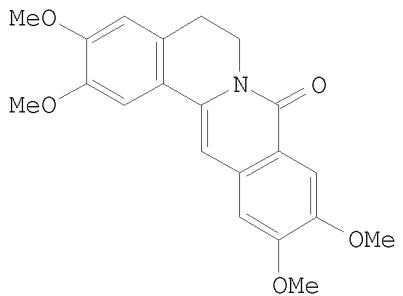
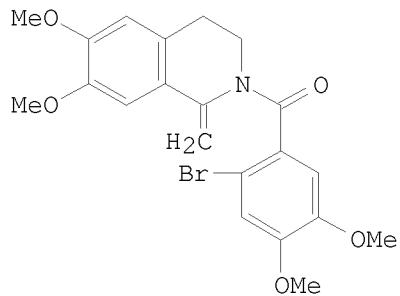
SOURCE: Heterocycles (1976), 4(5), 927-32

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

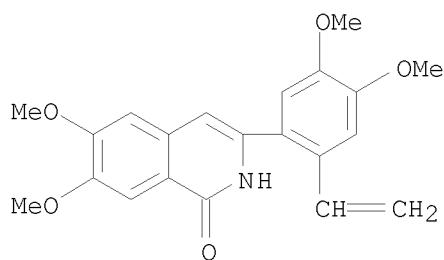


AB Enamide I, obtained by the condensation of
3,4-dihydro-6,7-dimethoxy-1-methylisoquinoline and
2-bromo-4,5-dimethoxybenzoyl chloride, was cyclized using NaNH₂-NH₃(l) to
give 15% oxoberbine II. Successive treatment of II with POCl₃ and reduction
using NaBH₄ gave (\pm)-xylopinine (III). Photolysis of I also gave II.

IT 60315-12-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 60315-12-0 HCAPLUS

CN 1(2H)-Isoquinolinone, 3-(2-ethenyl-4,5-dimethoxyphenyl)-6,7-dimethoxy-
(CA INDEX NAME)

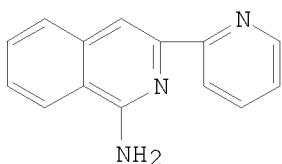


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 199 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1976:145358 HCAPLUS
DOCUMENT NUMBER: 84:145358
ORIGINAL REFERENCE NO.: 84:23589a,23592a

STN

TITLE: The growth-inhibitory action of some 1-aminoisoquinolines and related compounds on mycoplasma gallisepticum
AUTHOR(S): Van der Goot, Henderikus; Oostendorp, Joannes G.; Nauta, Wijbe T.
CORPORATE SOURCE: Dep. Med. Chem., Vrije Univ., Amsterdam, Neth.
SOURCE: European Journal of Medicinal Chemistry (1975), 10(6), 603-6
DOCUMENT TYPE: CODEN: EJMCA5; ISSN: 0223-5234
LANGUAGE: English
GI



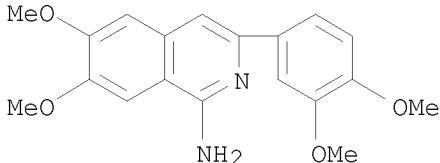
AB When a large number of 1-aminoisoquinolines was tested in vitro for activity against *M. gallisepticum*, the 3-(2-pyridyl) derivs. showed the highest activity, e.g., 1-amino-3-(2-pyridyl)isoquinoline (I) [37989-04-1]. 2,2'-Bipyridyl [366-18-7], 1,10-phenanthroline [66-71-7] and their derivs. were also tested. The lipophilicity of the compds. played a role in the activity; the mechanism of lipophilicity appears to be related to intercalation rather than complex formation.

IT 58814-54-3P

RL: PREP (Preparation)
(preparation and *Mycoplasma gallisepticum* inhibition by)

RN 58814-54-3 HCPLUS

CN 1-Isoquinolinamine, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)

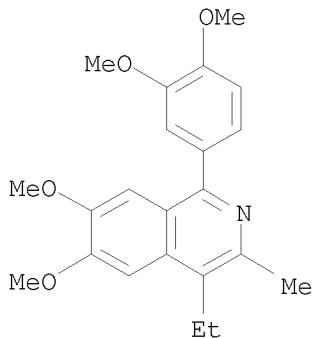


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 200 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1976:73232 HCPLUS
DOCUMENT NUMBER: 84:73232
ORIGINAL REFERENCE NO.: 84:12011a,12014a
TITLE: Isobenzopyrylium salts. VI. Carbon-13 NMR investigation of 1-arylnaphthalene derivatives and aza and oxa analogs

STN

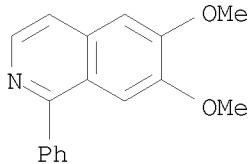
AUTHOR(S): Vajda, Miklos; Voelter, Wolfgang
CORPORATE SOURCE: Chem. Inst., Univ. Tuebingen, Tuebingen, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1975), 30B(11-12), 943-5
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 13C NMR spectra of 1-arylnaphthalenes, 1-arylisobenzpyrylium salts, N-methylisoquinolinium salts, and 1-arylisouinoline derivs. are determined
IT 1616-49-5
RL: PRP (Properties)
(carbon-13 NMR spectrum of)
RN 1616-49-5 HCPLUS
CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



L13 ANSWER 201 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1975:606075 HCPLUS
DOCUMENT NUMBER: 83:206075
ORIGINAL REFERENCE NO.: 83:32427a,32430a
TITLE: Action of periodic acid on isoquinoline derivatives
Side reactions observed in the oxidation of some
6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolines
Mahuzier, Georges; Hamon, Michel; Chaigneau, Marcel;
Gardent, Jean; Maitte, Pierre
AUTHOR(S): Mahuzier, Georges; Hamon, Michel; Chaigneau, Marcel;
Gardent, Jean; Maitte, Pierre
CORPORATE SOURCE: Fac. Sci. Pharm., Univ. Paris-Sud, Chatenay-Malabry,
Fr.
SOURCE: Analusis (1974), Volume Date 1973-1974,
2(9), 647-53
CODEN: ANLSCY; ISSN: 0365-4877
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The HIO₄ oxidation of I (R = Ph, R₁ = CO₂H, HOCH₂; R = H, R₁ = CO₂H, PhCHOH) gave the corresponding II (R = Ph, H) and MeOH via demethylation of III (R = Ph, H); the 6-MeO group was necessary for this reaction. II was further decomposed by HIO₄. The oxidation of IV [R = Ph, 3,4-(MeO)₂C₆H₃] gave RCO₂H and V; MeOH was not observed. Similar results were obtained with

STN

3,4-(MeO)2C6H3CHMeOH and 3,4-(MeO)2C6H3COMe.
IT 4029-09-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 4029-09-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)

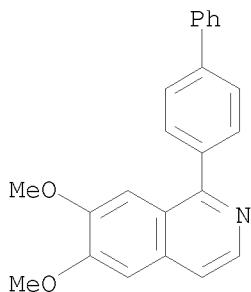


L13 ANSWER 202 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1975:458672 HCPLUS
DOCUMENT NUMBER: 83:58672
ORIGINAL REFERENCE NO.: 83:9251a,9254a
TITLE: 4-Biphenylyl isoquinoline derivatives
INVENTOR(S): Jansen, Alexander Bertus A.; Hollywood, John; Wilson, Alan Brian
PATENT ASSIGNEE(S): UK
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3823148	A	19740709	US 1972-256955	19720525 <--
GB 1386076	A	19750305	GB 1971-18765	19720602 <--
PRIORITY APPLN. INFO.:			GB 1971-18765	A 19710603

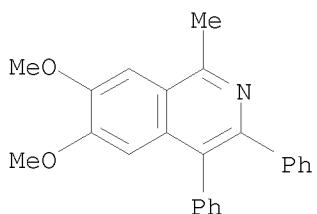
GI For diagram(s), see printed CA Issue.
AB The dihydroisoquinoline I (R = p-PhC6H4, 1-adamantyl, p-MeSO2NHC6H4CH2, p-H2NC6H4CH2, etc.; R1 = H, Me) were prepared by cyclization of amides. Thus, p-PhC6H4COCl was treated with 3,4-(MeO)2C6H3CH2CH2NH2 to give 3,4-(MeO)2C6H3CH2CH2NHCOC6H4Cl-p, which was cyclized with POCl3 to give I (R = p-PhC6H4, R1 = Me). Several I were reduced to the 1,2,3,4-tetrahydro derivs. I were hypotensives, depressants, and anticonvulsants (no data).

IT 56205-79-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56205-79-9 HCPLUS
CN Isoquinoline, 1-[1,1'-biphenyl]-4-yl-6,7-dimethoxy- (CA INDEX NAME)



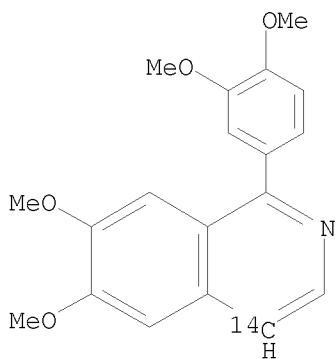
OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L13 ANSWER 203 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1975:125225 HCAPLUS
DOCUMENT NUMBER: 82:125225
ORIGINAL REFERENCE NO.: 82:20003a,20006a
TITLE: Formation of some isochromene derivatives during the reaction of veratryl ketones and veratric acid with benzoin
AUTHOR(S): Kuznetsov, E. V.; Pruchkin, D. V.; Bicherov, A. V.; Dorofeenko, G. N.
CORPORATE SOURCE: Rostov. Gos. Univ., Rostov-on-Don, USSR
SOURCE: Khimiya Geterotsiklichesikh Soedinenii (1974), (11), 1575
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Benzopyrylium perchlorates (I; R = Me, Ph, p-MeOC₆H₄) were obtained in 40-60% yields by heating 3,4-(MeO)₂C₆H₃COR with PhCH(OH)COPh in the presence of polyphosphoric acid 1 hr at 120-30°. Treatment of I with NH₄OAc gave isoquinolines (II). Treatment of veratric acid with benzoin similarly gave 12% isocoumarin (III) which could be transformed into I (R = Me) by MeMgI.
IT 27922-95-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27922-95-8 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)



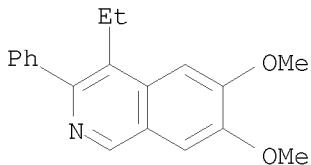
STN

L13 ANSWER 204 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1975:43625 HCPLUS
DOCUMENT NUMBER: 82:43625
ORIGINAL REFERENCE NO.: 82:6953a,6956a
TITLE: Synthesis of papaverine and quinopavine specifically labeled with carbon-14
AUTHOR(S): Ithakissios, S. D.; Tsatsas, G.; Nikokavouras, J.; Tsolis, A.
CORPORATE SOURCE: Nucl. Med. Lab., Minnesota Min. and Manuf. Co., St. Paul, MN, USA
SOURCE: Journal of Labelled Compounds (1974), 10(3), 369-79
CODEN: JLCAAI; ISSN: 0022-2135
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Papaverine labeled with ¹⁴C in either the benzyl or C-4 position and quinopavine labeled with ¹⁴C at the 1,4- or 4-methoxyphenyl position were synthesized. 3,4-Dimethoxybenzoic-carboxy-¹⁴C acid was the precursor in the synthesis of above compds. except for the 4-methoxyphenyl labeled where 3-methoxy-4-methoxy-¹⁴C-benzoic acid was employed. Reduction of 3,4-dimethoxybenzoyl-carbonyl-¹⁴C chloride gave 3,4-dimethoxybenzaldehyde-carbonyl-¹⁴C from which 2-(3,4-dimethoxyphenyl)-2-methoxyethylamine-2-¹⁴C was obtained through reduction of the corresponding ¹⁴C-labeled substituted nitrostyrene. 3,4-Dimethoxybenzoic-carboxy-¹⁴C acid was converted to (3,4-dimethoxyphenyl)acetonitrile-2-¹⁴C from which 2-(3,4-dimethoxyphenyl)ethylamine-2-¹⁴C was obtained on reduction and (3,4-dimethoxyphenyl)acetic acid-2-¹⁴C on alkaline hydrolysis. Heating at 200° the corresponding acids and amines, or a Schotten-Baumann reaction gave the corresponding amines which were cyclized in the presence of POCl₃. The 3,4-dihydro products were dehydrogenated. The cyclization of N-(3,4-dimethoxyphenyl-2-methoxyethyl-2-¹⁴C)-3,4-dimethoxyphenylacetamide gave the corresponding ¹⁴C-labeled papaverine.
IT 55323-26-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 55323-26-7 HCPLUS
CN Isoquinoline-4-¹⁴C, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (9CI) (CA INDEX NAME)



STN

L13 ANSWER 205 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:463463 HCPLUS
DOCUMENT NUMBER: 81:63463
ORIGINAL REFERENCE NO.: 81:10105a,10108a
TITLE: Preparation of substituted isoquinoline derivatives.
2
AUTHOR(S): Simon, L.; Talpas, G.
CORPORATE SOURCE: Pharm.-Chem. Inst., Szeged Med. Univ., Szeged, Hung.
SOURCE: Pharmazie (1974), 29(5), 314-16
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The isoquinoline I ($R = R_2 = H$, $R_1 = \text{CH}_2\text{Ph}$) was prepared by treating $\text{PhCH}_2\text{CH}_2\text{CO}_2\text{H}$ with $\text{o}-(\text{MeO})_2\text{C}_6\text{H}_4$, nitrosating the $3,4-(\text{MeO})_2\text{C}_6\text{H}_3\text{COCH}_2\text{CH}_2\text{Ph}$, reducing the $3,4-(\text{MeO})_2\text{C}_6\text{H}_3\text{CH}(\text{OH})\text{CH}(\text{NH}_2)\text{CH}_2\text{Ph}$, N-formylating, and cyclizing with POCl_3 . I ($R = H$, $R_1 = \text{Ph}$, $R_2 = \text{Et}$; $R = \text{Me}$, $R_1 = \text{Ph}$, $R_2 = H$) were similarly prepared. I ($R = R_2 = H$, $R_1 = \text{CH}_2\text{Ph}$) was a tranquilizer, whereas the other 2 compds. were inactive.
IT 52947-31-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52947-31-6 HCPLUS
CN Isoquinoline, 4-ethyl-6,7-dimethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 206 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:449547 HCPLUS
DOCUMENT NUMBER: 81:49547
ORIGINAL REFERENCE NO.: 81:7911a,7914a
TITLE: Cyclization reactions of
1,2-bis(2-cyanophenyl)propionitriles. II. Synthesis
of 5-amino-4,7-dimethoxy-11H-indeno[1,2-c]isoquinolin-
11-one
AUTHOR(S): Ando, Kazuo; Tokoroyama, Takashi; Kubota, Takashi
CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1974), 47(4), 1014-17
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The structure of 5-amino-4,7-dimethoxy-11H-indeno[1,2-c]isoquinolin-11-one (I) was confirmed by synthesis.

STN

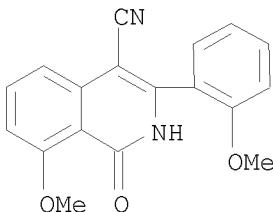
5,6-Dihydro-4,7-dimethoxy-11H-indeno[1,2-c]isoquinoline-5,11-dione (II) obtained from I was converted into I by chlorination with POCl_3 treatment with NH_3 . II was synthesized from 2-(2-carboxy-3-methoxyphenyl)-4-methoxyindan-1,3-dione via 4,7-dimethoxy-11H-indeno[1,2-c]isocoumarin-11-one.

IT 53015-02-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 53015-02-4 HCAPLUS

CN 4-Isoquinolinecarbonitrile, 1,2-dihydro-8-methoxy-3-(2-methoxyphenyl)-1-oxo- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L13 ANSWER 207 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:425573 HCAPLUS
DOCUMENT NUMBER: 81:25573
ORIGINAL REFERENCE NO.: 81:4125a, 4128a
TITLE: Antidiabetic 6-alkoxy-2-alkylisoquinolinium salts
INVENTOR(S): Garside, Peter; Dimsdale, Michael J.
PATENT ASSIGNEE(S): Allen and Hanburys Ltd.
SOURCE: Ger. Offen., 25 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

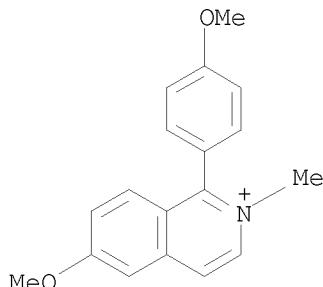
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2351184	A1	19740502	DE 1973-2351184	19731011 <--
GB 1407685	A	19750924	GB 1972-48211	19721019 <--
ZA 7307712	A	19740828	ZA 1973-7712	19731002 <--
AU 7361235	A	19750410	AU 1973-61235	19731010 <--
BE 806131	A1	19740416	BE 1973-136736	19731016 <--
AT 7308783	A	19760315	AT 1973-8783	19731016 <--
AT 333283	B	19761110		
CA 1019743	A1	19771025	CA 1973-183479	19731016 <--
NL 7314378	A	19740423	NL 1973-14378	19731018 <--
FR 2203629	A1	19740517	FR 1973-37198	19731018 <--
JP 49132081	A	19741218	JP 1973-117362	19731018 <--
DK 134013	B	19760830	DK 1973-5646	19731018 <--
CH 598224	A5	19780428	CH 1973-14722	19731018 <--
SE 402286	C	19781012	SE 1973-14205	19731018 <--

STN

US 4042697 A 19770816 US 1975-632577 19751117 <--
PRIORITY APPLN. INFO.: GB 1972-48211 A 19721019
US 1973-405120 A1 19731010

GI For diagram(s), see printed CA Issue.
AB About 40 salts I [X- = e.g. Cl, Br, iodide, HSO4, or O3SC6H4Me-4; R = e.g. H, C1-5 alkyl, allyl, CH2C.tplbond.CH, CH2CH2OPh, (CH2)3OMe, CH2CH2NH2, CH2Ph, cyclopentyl, or tetrahydro-3-furyl; R1 = H, Me, Et, CH2Ph, or C6H4OMe-4; R2 = e.g. Me, Bu, allyl, CH2C.tplbond.CH, CH2CH2NET2, CH2COPh, or CH2CH2OPh; R3 = H or Me] or their hydrobromides, used as antidiabetics, were prepared in most part by quaternization of the appropriate isoquinolines with R2X or alkylation of I (R = H) with RX. Thus, 6-methoxyisoquinoline and PhCH2Br were refluxed in Me2CO to give I (X = Br, R = Me, R1 = R3 = H, R2 = CH2Ph). I (X = iodide, R = R2 = Me, R1 = R3 = H) was refluxed in 48% HBr to give I (X = Br, R = R1 = R3 = H, R2 = Me), which on refluxing with PhCH2Br in MeCN gave I (X = Br, R = CH2Ph, R1 = R3 = H, R2 = Me).

IT 52986-81-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52986-81-9 HCPLUS
CN Isoquinolinium, 6-methoxy-1-(4-methoxyphenyl)-2-methyl-, chloride (1:1)
(CA INDEX NAME)



● Cl-

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 208 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:405277 HCPLUS
DOCUMENT NUMBER: 79:5277
ORIGINAL REFERENCE NO.: 79:891a,894a
TITLE: Substituted 3-(hydroxymethyl)isoquinolines and their derivatives
INVENTOR(S): Valette, Raymond
PATENT ASSIGNEE(S): Laboratories Albert Rolland
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German

STN

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2246307	A1	19730329	DE 1972-2246307	19720921 <--
DE 2246307	C2	19821104		
FR 2154500	A1	19730511	FR 1972-32294	19720912 <--
BE 788984	A1	19730115	BE 1972-2052190	19720919 <--
CH 550173	A	19740614	CH 1972-13748	19720920 <--
GB 1400425	A	19750716	GB 1971-44240	19720920 <--
CA 990297	A1	19760601	CA 1972-152191	19720920 <--
US 3891654	A	19750624	US 1972-290813	19720921 <--
FI 49827	B	19750630	FI 1972-2607	19720921 <--
DK 131778	B	19750901	DK 1972-4656	19720921 <--
RO 60560	A1	19760915	RO 1972-72297	19720921 <--
NL 7212904	A	19730326	NL 1972-12904	19720922 <--
ZA 7206478	A	19730627	ZA 1972-6478	19720922 <--
AU 7246982	A	19740328	AU 1972-46982	19720922 <--
AT 7208176	A	19750115	AT 1972-8176	19720922 <--
AT 325785	B	19751110		
CS 165974	B2	19751222	CS 1972-6482	19720922 <--
IL 40412	A	19760430	IL 1972-40412	19720922 <--
			GB 1971-44240	A 19710922

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

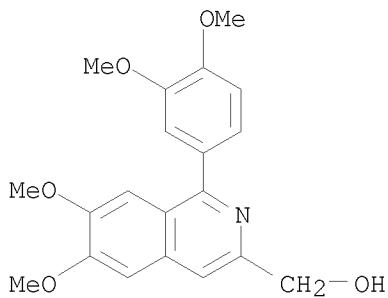
AB 1-Arylisooquinolines I ($R = 3,4-(MeO)2C_6H_3CH_2, 3,4-(EtO)2C_6H_3CH_2$, piperonyl, $3,4-(MeO)2C_6H_3$, $3,4,5-(MeO)3C_6H_2$, $3,4,5-(MeO)3C_6H_2CH_2CH_2$, 3-pyridyl, 2-thienyl, 2-furyl, 5-nitro-2-furyl; $R1 = H, Ac, COCH_2CH_2CO_2H, COCH_2CH_2Ph$; $R2 = Me, Et; R22 = CH_2$) were prepared. Thus, 3,4-dihydro-6,7-dimethoxy-3-(methoxycarbonyl)-1-(3,4-dimethoxybenzyl)isoquinoline was dehydrogenated and the methoxycarbonyl group reduced by $LiBH_4$ or $LiAlH_4$ to give I ($R = 3,4-(MeO)2C_6H_3CH_2, R1 = H, R2 = Me$), which was converted to its hemisuccinate with succinic anhydride. I are spasmolytics 25 times as effective as papaverine-HCl, and are approx. as effective as papaverine-HCl as coronary dilators.

IT 41599-02-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

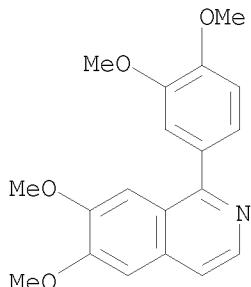
RN 41599-02-4 HCPLUS

CN 3-Isoquinolinemethanol, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



STN

L13 ANSWER 209 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:509309 HCPLUS
DOCUMENT NUMBER: 77:109309
ORIGINAL REFERENCE NO.: 77:17975a,17978a
TITLE: Cyclic nucleotide phosphodiesterase inhibition and vascular smooth muscle relaxation
AUTHOR(S): Lugnier, C.; Bertrand, Y.; Stoclet, J. C.
CORPORATE SOURCE: U.E.R. Sci. Pharm, Univ. Louis Pasteur, Strasbourg, Fr.
SOURCE: European Journal of Pharmacology (1972), 19(1), 134-6
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A quant. correlation was observed between the inhibition of 3',5'-cyclic nucleotide phosphodiesterase by theophylline [58-55-9], papaverine [58-74-2], eupaverin [1163-37-7], quinoparaine [6,7-dimethoxy-1-(3',4'-dimethoxyphenyl)isoquinoline-HCl] [36455-58-0], and 6,7-dimethoxy-4-p-chlorobenzylisoquinoline-HBr [32872-00-7] in the isolated rat aorta and the prevention of Ba-induced aortic contractions by these compds. The results are consistent with the hypothesis that phosphodiesterase inhibition and subsequent cyclic AMP accumulation play a role in the relaxing effect of these drugs on vascular smooth muscle.
IT 36455-58-0
RL: BIOL (Biological study)
(muscle relaxation by, cyclic nucleotide phosphodiesterase inhibition in)
RN 36455-58-0 HCPLUS
CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-, hydrochloride (1:1)
(CA INDEX NAME)



● HCl

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

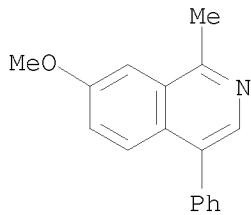
L13 ANSWER 210 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:475145 HCPLUS
DOCUMENT NUMBER: 77:75145
ORIGINAL REFERENCE NO.: 77:12415a,12418a

STN

TITLE: 4-Phenylisoquinolines
INVENTOR(S): Grethe, Guenter; Uskokovic, Milan Radoje
PATENT ASSIGNEE(S): Hoffman-La Roche Inc.
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3666763	A	19720530	US 1970-1062	19700106 <--
PRIORITY APPLN. INFO.:			US 1970-1062	A 19700106

GI For diagram(s), see printed CA Issue.
AB 4-Aryltetrahydroisoquinolines (I, R = H, Me, R1 = H, Me, PhCH2; R2 = Ph, p-MeC6H4; R3 = Cl, HO, MeO; R4 = H) useful as antidepressants and hypotensive agents were prepared (chiefly as HCl salts) by reductive alkylation of di-hydroisoquinolones and hydrogenolysis of the tertiary OH groups. Some I were also resolved. Thus, 3 g Mg and 22 g PhBr in THF were treated with 25 g 2-benzyl-2,33-dihydro-7-methoxy-4(1H)-isoquinolone to give 32 g I.HCl (R = H, R1 = PhCH2, R2 = Ph, R3 = MeO, R4 = HO). Hydrogenation of 5.6 g I (R = H, R1 = PhCH2, R2 = Ph, R3 = MeO, R4 = HO) over Pd-C in HOAc at 60° and 50 psi, followed by HCl-Me2-CHOH gave I.HCl (R = H, R1 = H, R2 = Ph, R3 = MeO, R4 = H). Alternately acid dehydration of the isoquinolinol with disproportionation of the dihydro product and metal hydride reduction of the isoquinoline gave I. I.HCl (R = H, Me; R1 = Me; R2 = Ph; R3 = MeO; R4 = H) had ED50 of 1.0 and 0.5 mg/kg resp. in the ptosis-anti-tetrabenazine test.
IT 37624-20-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 37624-20-7 HCPLUS
CN Isoquinoline, 7-methoxy-1-methyl-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

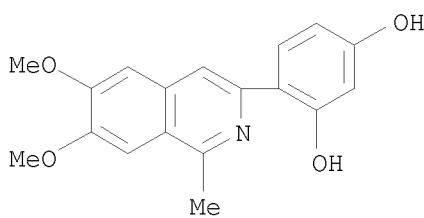
L13 ANSWER 211 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:140418 HCPLUS

STN

DOCUMENT NUMBER: 76:140418
ORIGINAL REFERENCE NO.: 76:22779a, 22782a
TITLE: 2-Benzopyrylium salts. VII. Synthesis of
6,7-dimethoxy-2-benzopyrlium salts and isoquinolines
with aromatic substituents in the 3-position
AUTHOR(S): Dorofeenko, G. N.; Kuznetsov, E. V.
CORPORATE SOURCE: USSR
SOURCE: Khim. Geterotsikl. Soedin. (1970), No. 2,
207-12
From: Ref. Zh., Khim. 1971, Abstr. No. 6Zh753
DOCUMENT TYPE: Journal
LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.
AB Unspecified R = H throughout. A mixture of 0.01 mole veratrole and 0.11
mole homoveratric acid (I) was heated at 100° until nonhomogeneous,
20 g polyphosphoric acid (PPA) added, and the mixture stirred 2 hr at
100° to give 87% II (R1 = R2 = OMe) (IIa). Similarly prepared was
93% II (R2 = OMe). IIa (3 mmoles) and 3.1 mmoles I heated until
nonhomogeneous, 10 g PPA added, and the mixture stirred 1.5 hr at
100° gave 82% II [R1 = R2 = OMe, R2 = 3,4-(MeO)2C6H3CH2CO] (IIb).
Similarly prepared were 66% II [R1 = R2 = OMe, R3 = 3,4-(MeO)2C6H3CO] and
89% II (R1 = R2 = OMe, R3 = PhCH2CO). IIa (0.4 g) was dissolved in 5 ml
Ac2O, 0.3 ml 70% HClO4 added, and the mixture kept 24 hr to give 86% III (R1
= R2 = OMe, R3 = Me). Similarly prepared III were (R, R1, R2, R3, and %
yield given): H, OMe, OMe, Et, 94; H, OMe, OMe, Pr, 83; H, H, OMe, OMe,
83; H, OMe, OMe, 3,4-(MeO)2C6H3CH2 (IIIa), 94; H, OMe, OMe, PhCH2, 96; H,
OMe, OMe, 3,4-(MeO)2C6H3, 98; OAc, H, OAc, Me (IIIb), 78; OAc, H, OMe, Me,
68; OH, H, OMe, Et, 80; OMe, H, OMe, Me, 70; OH, H, OH, Me, 86; and OH,
H, OMe, Me, 77. Through a suspension of 0.35 g IIIb in 2.5 ml alc. was
passed NH3; the salt dissolved, and 82% IV (R = R2 = OH, R3 = Me) precipitated.
Similarly prepared was 80% IV (R = OH, R2 = MeO, R3 = Me). A suspension of
0.2 g IIIa in 5 ml alc. was saturated with NH3 at -10° in an ampul, and
the ampul sealed and heated 6 hr at 100° to give 80% IV [R1 = R2 =
MeO, R3 = 3,4-(MeO)2C6H3CH2]. Similarly prepared was 75% IV (R1 = R2 = MeO,
R3 = Me).
IT 35989-90-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

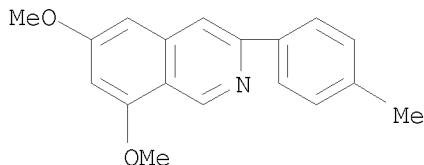
RN 35989-90-3 HCPLUS
CN 1,3-Benzenediol, 4-(6,7-dimethoxy-1-methyl-3-isoquinolinyl)- (CA INDEX
NAME)



L13 ANSWER 212 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:3663 HCPLUS
DOCUMENT NUMBER: 76:3663

STN

ORIGINAL REFERENCE NO.: 76:643a,646a
TITLE: Chemistry of fungi. LXVI. New synthesis of isoquinolines
AUTHOR(S): Ahmad, S.; Whalley, W. B.; Jones, D. F.
CORPORATE SOURCE: Sch. Pharm., London, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (21), 3590-3
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 76:3663
GI For diagram(s), see printed CA Issue.
AB The Gattermann aldehyde synthesis (HCN-ZnCl₂-HCl) applied to 3,5-dimethoxy- (I) or 3,5-dihydroxybenzyl ketones (II) gave 3-substituted 6,8-dimethoxy- or 6,8-dihydroxyisoquinolines (III; R₁ = Me, Et, Me₂CH, Bu, or p-tolyl), resp.
IT 34489-54-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34489-54-8 HCAPLUS
CN Isoquinoline, 6,8-dimethoxy-3-(4-methylphenyl)- (CA INDEX NAME)

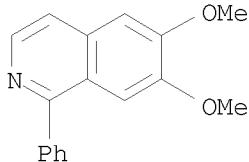


OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

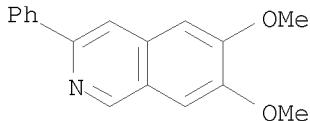
L13 ANSWER 213 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1971:529637 HCAPLUS
DOCUMENT NUMBER: 75:129637
ORIGINAL REFERENCE NO.: 75:20463a,20466a
TITLE: Oxidation of 1-phenyl-1-carboxy-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline by periodic acid
AUTHOR(S): Mahuzier, Georges; Hamon, Michel; Gardent, Jean;
Chaigneau, Marcel
CORPORATE SOURCE: Lab. Chim. Anal., CNRS, Paris, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1971), 273(4), 346-8
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The title process consumed abnormal amts. of HIO₄ and gave I, small amts. of secondary products, CO₂, and MeOH. The abnormal consumption of HIO₄ was caused by reaction with the MeO groups in the title compound
IT 4029-09-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

STN

RN 4029-09-8 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 214 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1971:111885 HCAPLUS
DOCUMENT NUMBER: 74:111885
ORIGINAL REFERENCE NO.: 74:18124h,18125a
TITLE: Synthesis of isoquinolines from (benzylamino)acetonitriles. 1. Compounds prepared from veratrylamine
AUTHOR(S): Waigh, R. D.; Harcourt, D. N.
CORPORATE SOURCE: Dep. Pharm. Chem., Univ. Strathclyde, Glasgow, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (5), 967-70
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 74:111885
GI For diagram(s), see printed CA Issue.
AB [(3,4-Dimethoxybenzyl)amino]acetonitriles (I) cyclized in concentrated H₂SO₄ to give, after hydrolysis, 24-83% 1,2-dihydro-4(3H)-isoquinolinones (II). 3,3-Disubstituted 1,2-dihydro-4(3H)-isoquinolinones (e.g. II, R₁ = R₂ = Me) were stable as the free base, in contrast to the 3-unsubstituted and 3-monosubstituted analogs. II (R₁ = Ph, R₂ = H) underwent air oxidation to give 6,7-dimethoxy-3-phenyl-4-isoquinolinol; II was also converted into 6,7-dimethoxy-3-phenylisoquinoline.
IT 24285-10-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24285-10-7 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-3-phenyl- (CA INDEX NAME)

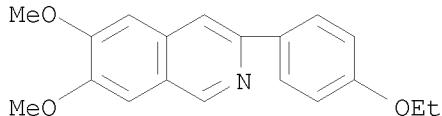


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

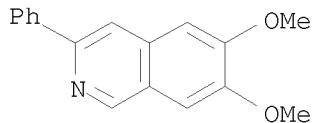
L13 ANSWER 215 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1971:76295 HCAPLUS
DOCUMENT NUMBER: 74:76295
ORIGINAL REFERENCE NO.: 74:12379a,12382a

STN

TITLE: Synthesis of 3-aryl derivatives of 2-benzopyrylium salts with free α -positions
AUTHOR(S): Dorofeenko, G. N.; Safaryan, G. P.; Kuznetsov, E. V.
CORPORATE SOURCE: Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR
SOURCE: Khimiya Geterotsiklichesikh Soedinenii (1970)
(8), 1013-14
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Benzopyrylium salts (I) were prepared Homoveratric acid, PhOEt, and polyphosphoric acid was heated 2 hr at 65° to give II (Ar = C₆H₄OEt-p) (III). III, AlCl₃, and Cl₂CHOBu in CH₂Cl₂ was kept 10 min and worked up with 70% HClO₄ to give I (Ar = C₆H₄-OEt-p). Similarly prepared were 3 other I compds. I (Ar = p-EtO-C₆H₄) and 22% aqueous NH₃ kept 3 days gave IV (Ar = C₆H₄OEt-p).
IT 30748-36-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30748-36-8 HCPLUS
CN Isoquinoline, 3-(4-ethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



L13 ANSWER 216 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1971:3574 HCPLUS
DOCUMENT NUMBER: 74:3574
ORIGINAL REFERENCE NO.: 74:581a,584a
TITLE: Reactions of benzylcarbonyl compounds with formamide.
VII. Reactions of deoxybenzoins
AUTHOR(S): Koyama, Takaji; Katsuse, Yoshiki; Toda, Mutsuko;
Hirota, Takashi; Yamato, Masatoshi
CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Kunmamoto, Kumamoto, Japan
SOURCE: Yakugaku Zasshi (1970), 90(10), 1207-11
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB 4,5-Diphenylpyrimidine was obtained on heating deoxybenzoin with HCONH₂ and POCl₃. Several deoxybenzoins were reacted to define this preparative method.
IT 24285-10-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24285-10-7 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 217 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1970:509706 HCAPLUS
DOCUMENT NUMBER: 73:109706
ORIGINAL REFERENCE NO.: 73:17859a,17862a
TITLE: Pharmacologically active
2-amino-1-(3,4-dimethoxyphenyl)-4-ethyl-3-methyl-6,7-dimethoxyisoquinolinium hydroxide inner salt
PATENT ASSIGNEE(S): Egyesult Gyogyszer es Tapszergyar
SOURCE: Brit., 4 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1202579	---	19700819	GB 1967-55088	19671204 <--
DE 1670462			DE	
DE 1670642			DE	
FR 6852			FR	
US 3736315		19730529	US	19710304 <--
PRIORITY APPLN. INFO.:			HU	19661209

GI For diagram(s), see printed CA Issue.

AB The title compound (I) is a tranquilizing agent about 5 times as active per os as meprobamate in animal tests. Refluxing a mixture of 38.64 g 3,3',4,4'-tetramethoxy-6-(α -acetylpropyl)benzophenone (II), 15 g 100% N2H4.H2O, and 200 ml EtOH for 3 hr and cooling gave 24.8 g 1-hydrazino-1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxy-1H-2-benzopyran (III), m. 136°, contaminated with some 1-(3,4-dimethoxyphenyl)-4-methyl-5-ethyl-7,8-dimethoxy-5H-2,3-benzodiazepine (IV), m. 136° (iso PrOH). IV results from splitting out H2O from III, a spontaneous process slow in EtOH at 25° and more rapid on heating. Refluxing a mixture of 38.6 g II, 5.5 g N2H4.H2O, and 500 ml EtOH 5 hr, adding 100 ml C6H6, and distilling 400 ml solvent during 3 hr gave 19 g IV. Heating III at 150°/10 mm until loss of H2O ceased also gave IV; picrate m. 184-5°. A solution of 0.01 mole III containing some IV in 20 ml MeOH saturated with dry HCl was evaporated

and treated with 20 ml 5% NaOH to give I.H2O, m. 95-115°. The anhydrous product was obtained, m. 156-7° (2.7 g), by crystallization from iso-PrOH. I.HCl m. 217.5°; I picrate m. 204°. I (2.55 g) was prepared in one stage from 3.86 g II, 0.011 mole N2H4.H2O, 60 ml EtOH, and 0.005 mole H2SO4 by refluxing 10 hr. Treating 4.41 g 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisobenzopyrylium chloride-HCl in 3k ml MeOH at 20-5° with 0.75 g N2H4.H2O in 5 ml MeOH, evaporating, and stirring with 3 ml H2O gave 3.3 g I.HCl. A mixture of

STN

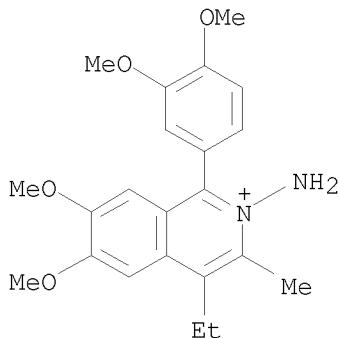
9.18 g 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisoquinoline, 2.8 g KCN, 60 ml H₂O, and 2.82 g hydrosylamine-O-sulfonic acid was heated at 80° for 2 hr to give 70% I.

IT 1092167-62-8P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Pharmacologically active 2-amino-1-(3,4-dimethoxyphenyl)-4-ethyl-3-methyl-6,7-dimethoxyisoquinolinium hydroxide inner salt)

RN 1092167-62-8 HCPLUS

CN Isoquinolinium, 2-amino-1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl-, hydroxide (1:1) (CA INDEX NAME)



● OH⁻

L13 ANSWER 218 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1970:445480 HCPLUS

DOCUMENT NUMBER: 73:45480

ORIGINAL REFERENCE NO.: 73:7507a,7510a

TITLE: Quinazolines and 1,4-benzodiazepines. XLV.
1,4-Benzodiazepines from 4-isooquinolinones

AUTHOR(S): Fryer, Rodney I.; Earley, James V.; Evans, E.;
Schneider, J.; Sternbach, Leo H.

CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ,
USA

SOURCE: Journal of Organic Chemistry (1970), 35(7),
24559

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

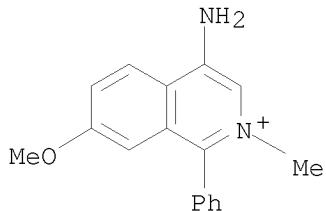
AB 1,2,3,4-Tetrahydro-4-isooquinolinones (I) are treated with NaN₃ to give 1,3,4,5-tetrahydro-2H-1,4-benzodiazepin-2-ones (II). II are also prepared from I oximes and polyphosphoric acid.

IT 24781-77-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24781-77-9 HCPLUS

CN Isoquinolinium, 4-amino-7-methoxy-2-methyl-1-phenyl-, chloride (1:1) (CA INDEX NAME)



● Cl⁻

L13 ANSWER 219 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1970:132239 HCPLUS

DOCUMENT NUMBER: 72:132239

ORIGINAL REFERENCE NO.: 72:23667a,23670a

TITLE: Use of polyphosphoric acid in the synthesis of
ω,ω-diaryl-substituted acetophenones;
3,4-diaryl-substituted 2-benzopyrylium salts and
isoquinolines based on them

AUTHOR(S): Kuznetsov, E. V.; Dorofeenko, G. N.

CORPORATE SOURCE: Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1970), 6(3),
578-81

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

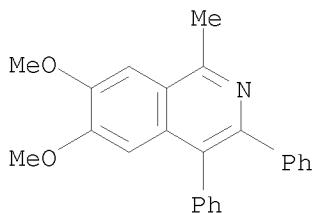
AB Condensation of veratrole with BZCH(OH)Ph, PhCH(OH)CO₂H, or BZCHO in polyphosphoric acid gave 62-8% 3,4-(MeO)2C₆H₃-CHRCOR1 (I) (R, R1 given): Ph, Ph; Ph, 3,4-(MeO)2C₆H₃; 3,4-(MeO)2C₆H₃, Ph; resp. Heating I (R = R1 = Ph) with Ac₂O and HClO₄ gave 6,7-dimethoxy-3,4-diphenyl-1-methyl-2-benzopyrylium perchlorate. Similarly, 6,7-dimethoxy-1,3,4-triphenyl-2-benzopyrylium and 6,7-dimethoxy-1-benzyl-3,4-diphenyl-2-benzopyrylium perchlorates were prepared 6,7-Dimethoxy-3,4-diphenyl-1-methylisoquinoline, and 1-benzyl-6,7-dimethoxy-3,4-diphenylisoquinoline were prepared from NH₃ and the resp. perchlorate.

IT 27922-95-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

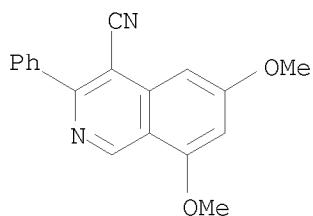
RN 27922-95-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

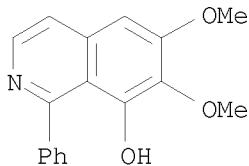
L13 ANSWER 220 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1970:55204 HCPLUS
DOCUMENT NUMBER: 72:55204
ORIGINAL REFERENCE NO.: 72:10089a,10092a
TITLE: Reactions of benzylcarbonyl compounds with formamide.
II. A novel synthesis of isoquinolines
AUTHOR(S): Toyama, Takaji; Hirota, Takashi; Ito, Itsuya; Toda,
Mutsuko; Yamato, Masatoshi
CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Kumamoto, Kumamoto, Japan
SOURCE: Yakugaku Zasshi (1969), 89(11), 1492-5
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI For diagram(s), see printed CA Issue.
AB Treating 3,5-dimethoxyphenylacetonitrile (I) with Me₂NCHO and POCl₃ under the usual conditions of the Vilsmeier reaction gave 3-chloro-6,8-dimethoxyisoquinoline (II). Although II had already been synthesized from I by the Gattermann reaction, its formation from I by the Vilsmeier reaction had not been described. Under the conditions of the Vilsmeier reaction modified by using H₂NCHO, 2-(3,5-dimethoxyphenyl)-5-(4-methoxyphenyl)-3-oxopentanonitrile gave 4-isoquinolinecarbonitriles (III and IV). The formation of IV may proceed through the elimination of the acyl group, since 4-methoxydihydrocinnamamide was isolated from the reaction. Several other α -acyl-3,5-dimethoxy-phenylacetonitriles were used to generalize this direct isoquinoline synthesis, and the corresponding 4-isoquinolinecarbonitriles obtained without any acyl group elimination. In some cases, enamines were isolated as by-products.
IT 19713-14-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19713-14-5 HCPLUS
CN 4-Isoquinolinecarbonitrile, 6,8-dimethoxy-3-phenyl- (CA INDEX NAME)



STN

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 221 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1970:3472 HCAPLUS
DOCUMENT NUMBER: 72:3472
ORIGINAL REFERENCE NO.: 72:639a,642a
TITLE: Syntheses of heterocyclic compounds. CCCXX.
Syntheses of 1-substituted isoquinolines and
1,4-benzoxazepine derivatives by Pomeranz-Fritsch
reaction
AUTHOR(S): Kametani, Tetsuji; Ohkubo, Kazumi; Takano, Seiichi
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, Japan
SOURCE: Yakugaku Zasshi (1969), 89(8), 1048-55
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI For diagram(s), see printed CA Issue.
AB Since I is well known as a peripheral vasodilator agent, synthesis of its benz[e][1,4]oxazepine derivs. was carried out in order to exam. their activities. Furthermore, 1-benzylisoquinoline derivs. as well as 1,4-benzoxazepine derivs. had not yet been obtained by Pomeranz-Fritsch reaction with H₂SO₄ as condensing reagent. It was established that 1-benzylisoquinolines (II-V) as by-products and benz[e][1,4]oxazepine derivs. (VI-IX) can be obtained by Pomeranz-Fritsch reaction with polyphosphoric acid. In addition, cyclization of X with polyphosphoric acid gave debrominated 1-benzylisoquinoline together with 1,4-benzoxazepine derivative XI. Although cyclization of 2,3,4-(HO)(MeO)2C₆H₂COMe and 2,3,4-(HO)(MeO)2C₆H₂COPh afforded 1-benzylisoquinoline derivs. (XII and XIII), the expected 1,4-benzoxazepine derivs. (XIV and XV) were not obtained in both cases.
IT 24852-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24852-47-9 HCAPLUS
CN 8-Isoquinolinol, 6,7-dimethoxy-1-phenyl-, hydrochloride (1:1) (CA INDEX
NAME)



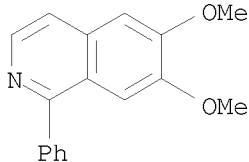
● HCl

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 222 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:481114 HCAPLUS

STN

DOCUMENT NUMBER: 71:81114
ORIGINAL REFERENCE NO.: 71:15016h, 15017a
TITLE: Organic photochemistry. I. 3,4-Dihydroisoquinolines from tetrahydroisoquinoline N-tosylates
AUTHOR(S): Umezawa, Bunsuke; Hoshino, Osamu; Sawaki, Shohei
CORPORATE SOURCE: Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1969), 17(6), 1115-19
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Photolysis of 1-substituted-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline N-tosy derivs. (I, R = H, Me, Ph, or CH₂Ph; Ts = tosyloxy) with high pressure Hg lamps (100-w. and 400-w.) in neutral (EtOH) or basic (80% by volume EtOH containing Na₂CO₃) media was examined. Under these conditions, 3,4-dihydro compounds (II, R = same as above) were formed in moderate yields.
IT 4029-09-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 4029-09-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)

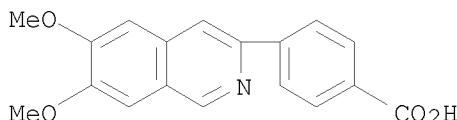


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L13 ANSWER 223 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:470474 HCPLUS
DOCUMENT NUMBER: 71:70474
ORIGINAL REFERENCE NO.: 71:13009a, 13012a
TITLE: 3-Aryl-isoquinoline derivatives
AUTHOR(S): Szabo, Janos; Vinkler, Elemer; Simon, Lajos; Varga, Istvan
CORPORATE SOURCE: Szegedi Orvostud. Egy., Szeged, Hung.
SOURCE: Acta Pharmaceutica Hungarica (1969), 39(3), 97-105
CODEN: APHGAO; ISSN: 0001-6659
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI For diagram(s), see printed CA Issue.
AB Several attempts were made to prepare 3-(4-carboxyphenyl)-6,7-dimethoxyisoquinoline (I). p-NCC₆H₄CH₂CN and an equivalent amount EtNO₂ were condensed in alc. in the presence of an equivalent amount EtONa to give 72% p-NCC₆H₄C(CN):N(O)ONa, which on reaction with aqueous NaOH provided 44% p-HO₂CC₆H₄-CH₂NO₂ (II), m. 183-4° (aqueous alc.). II was converted to its acyl chloride with SOC₁₂ which was then esterified with alc.-pyridine

to the Et ester (III), m. 70-2° (aqueous alc.), in 58% yield. Condensation of III with veratraldehyde failed. As a model to I, 3-phenyl-6,7-dimethoxyisoquinoline (IV) was synthesized by a new method. 3,4-(MeO)2C6H3COCH2Ph was nitrosated with a small excess of iso-C5H11NO2 in alc. in the presence of an equivalent amount of EtONa at 0° to 66% 3,4-(MeO)2C6H3COCPh:NOH (α -isomer), m. 151-3° (C6H6) (β -isomer m. 129-31°), which was hydrogenated in alc.-HCl over Pd/C to .apprx. 92% 3,4-(MeO)2(C6H3COCH-PhNH2.HCl (V), m. 223-4° (decomposition); N-benzoyl derivative m. 172-3° (alc.). V was reduced in aqueous alc. with Pd/C (73% yield) or with NaBH4 (80% yield) to 3,4-(MeO)2C6H3CH(OH)CH-PhNH2, m. 137-8.5° (alc.); N-benzoyl derivative m. 222-3° (C6H6). The formate of this amine was heated at 180° (oil bath) under vacuum for 20 min. and formed 67% 3,4-(MeO)2C6H3CH(OH)-CHPhNHCHO, m. 149.5-50°, which was refluxed 20 min. in PhMe with P2O5 to give 50% IV, m. 127-8° (50% aqueous alc.). Modifications of the above method served to prepare I. Thus, crude 4-NCC6H4CH2COCl (prepared from the acid with SOC12) and veratrol were dissolved in PhNO2 and, with cooling, anhydrous AlCl3 was added gradually. The mixture was kept 24 hrs. at room temperature and 20 min. at 60° to give 58% 3',4'-dimethoxy-4-cyanodeoxybenzoin (VI), m. 119-20.5° (alc.). VI was dissolved in refluxing absolute alc. and dry HCl gas was led in for 11 hrs. to give 92% 3',4'-dimethoxy-4-carbethoxydeoxybenzoin, m. 103-4° (alc.), which was treated with iso-C5H11NO2-EtONa in alc. at 0° for 24 hrs. to give 67% 3',4'-dimethoxy-4-carbethoxy- α -isonitrosodeoxybenzoin (VII), m. 139-40° (alc.); β -isomer m. 121-2°. VII was catalytically reduced to the amine, which, on reduction with NaBH4 at 0° formed 70% α -(3,4-dimethoxyphenyl)- β -(4-carbethoxyphenyl)- β -aminoethanol, m. 127-8.5° (alc.); a different modification m. 141-2°; N,O-dibenzoyl derivative m. 207-7.5° (C6H6). The formate of the amine on fusing at 180° gave 64% α -(3,4-dimethoxyphenyl)- β -(4-carbethoxyphenyl)- β -formylaminoethanol (VIII), m. 170-1° (alc.). Heating VIII with P2O5 failed to close the ring, giving 46% 3',4'-dimethoxy-4-carbethoxy-7-aminostilbene (IX), m. 173.5-75° (alc.). Ring closure occurred when VIII was refluxed with POCl3 for 15 min., leading to 55% 3-(4-carbethoxyphenyl)-6,7-dimethoxyisoquinoline, m. 178.5-9.5° (alc.), which on alc. KOH hydrolysis gave 89% I, m. 258-60° (alc.). II Na salt is ataractic.

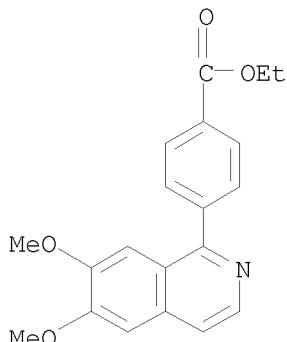
IT 24283-92-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 24283-92-9 HCPLUS
 CN Benzoic acid, 4-(6,7-dimethoxy-3-isoquinolinyl)- (CA INDEX NAME)



L13 ANSWER 224 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1969:461173 HCPLUS
 DOCUMENT NUMBER: 71:61173

STN

ORIGINAL REFERENCE NO.: 71:11251a,11254a
TITLE: 1-Aryl-isoquinoline derivatives
AUTHOR(S): Szabo, Janos; Simon, Lajos; Vinkler, Elemer
CORPORATE SOURCE: Szegedi Orvostud. Egy., Szeged, Hung.
SOURCE: Acta Pharmaceutica Hungarica (1969), 39(3),
106-9
CODEN: APHGAO; ISSN: 0001-6659
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI For diagram(s), see printed CA Issue.
AB The Bischler-Napieralski isoquinoline synthesis was employed to prepare 1-(4-carboxyphenyl)-6,7-dimethoxyisoquinoline (I). 3,4-(MeO)2C6-H3CH2CH2NH2 was condensed with 4-NCC6H4COCl in ether at room temperature to give 80% N-(4-cyanobenzoyl)-β-(3,4-dimethoxyphenyl)ethylamine, m. 122-3.5° (alc.), which, refluxed 6 hrs. in absolute alc. containing dry HCl gas gave 93% N-(4-carbethoxybenzoyl)-β-(3,4-dimethoxyphenyl)ethylamine (II), m. 167-9° (alc.). Ring closure of II was effected in refluxing POC13 (20 min.) to give 1-(4-carbethoxyphenyl)-6,7-dimethoxy-3,4-dihydroisoquinoline (III), m. 127-9° (alc.) and an unidentified compound, m. 106-9°, in 5:1.4 ratio. III was dehydrogenated by heating at 170° (oil bath) with Pd/C 30 min. to yield 1-(4-carboxyphenyl)-6,7-dimethoxyisoquinoline, m. 134-5° (alc.), which, on aqueous-alc. KOH hydrolysis gave I, m. 249-50° (decomposition) (alc.); morpholide m. 72-5° (or 87-9° from H2O). I and its morpholide possess ataractic action.
IT 23581-36-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23581-36-4 HCPLUS
CN Benzoic acid, 4-(6,7-dimethoxy-1-isoquinolinyl)-, ethyl ester (CA INDEX NAME)



L13 ANSWER 225 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:439240 HCPLUS
DOCUMENT NUMBER: 71:39240
ORIGINAL REFERENCE NO.: 71:7255a,7258a
TITLE: Norcoralydine
AUTHOR(S): Dutta, N. L.; Wadia, M. S.; Bindra, A. A.
CORPORATE SOURCE: Nat. Chem. Lab., Poona, India

STN

SOURCE: Indian Journal of Chemistry (1969), 7(5),
527
CODEN: IJOCAP; ISSN: 0019-5103

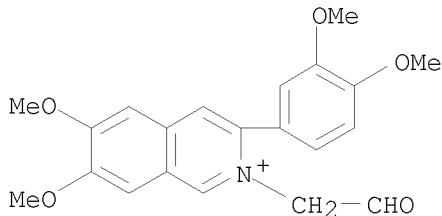
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.
AB A three-step synthesis of norcoralydine (I), starting from 3-(3,4-dimethoxyphenyl)-6,7-di-methoxyisoquinoline, is described. The steps are: (1) quaternization with bromoacetaldehyde; (2) treatment with HCl to yield a cyclized product; and (3) hydrogenation of the resulting cyclized product to (\pm)-I.

IT 23158-18-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23158-18-1 HCPLUS

CN Isoquinolinium, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-2-(2-oxoethyl)-, bromide (1:1) (CA INDEX NAME)



● Br⁻

L13 ANSWER 226 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:413034 HCPLUS
DOCUMENT NUMBER: 71:13034
ORIGINAL REFERENCE NO.: 71:2387a,2390a
TITLE: Aminoisoquinolines
PATENT ASSIGNEE(S): N. V. Koninklijke Pharmaceutische Fabrieken Voorheen Brocades-Stheeman & Pharmacia
SOURCE: Neth. Appl., 12 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
NL 6808726		19681223	NL 1968-8726	19680621 <--
DE 1770670			DE	
FR 1579053			FR	
FR 7723			FR	
GB 1173227			GB	
PRIORITY APPLN. INFO.:			GB	19670622

STN

OTHER SOURCE(S): MARPAT 71:13034

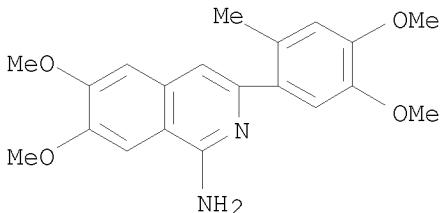
AB Title compds. are prepared from a substituted benzonitrile, a strongly basic alkali-metal compound, and a nitrile, followed by reaction with H₂O; they have depressive and spasmolytic properties. Thus, to a solution of 32 g. PhBr and 2.8 g. Li in 150 ml. anhydrous Et₂O 20 g. (iso-Pr)₂NH in 30 ml. Et₂O is added dropwise under N, followed by 26.2 g. 2,6-Me₂C₆H₃CN in 200 ml. C₆H₆. The mixture is refluxed 1 hr. and worked up to yield 11 g. 1-amino-8-methyl-3-(2,6-xylyl)isoquinoline, m. 187-8° [petroleum ether (b. 80-100°)-C₆H₆]; HCl salt m. 235-9° and 263-5° (EtOH); both forms have the same ir and N.M.R. spectra. To a solution of 8 g. K and some crystals of Fe(NO₃)₃·9H₂O in 300 ml. liquid NH₃ under N is added a solution of 11.7 g. o-tolunitrile in Et₂O. After 15 min., a solution of 20.6 g. PhCN in Et₂O is added, and the mixture kept overnight at room temperature and worked up to yield 56% 1-amino-3-phenylisoquinoline, m. 95-6° (CHCl₃-petroleum ether). Similarly are prepared 25% 1-amino-3-tert-butyliisoquinoline-HCl, sublimes >300° (EtOH); 45% 1-amino-3-(4,5-dimethoxy-o-tolyl)-6, 7-dimethoxyisoquinoline, m. 190-1.5° (CHCl₃-petroleum ether); 60% 1-amino-3-(o-tolyl)isoquinoline, m. 123.5-4.5°; and 20% 1-amino-3-(o-ethylphenyl)-4-methylisoquinoline-HCl m. apprx. 270° (decomposition) (EtOH).

IT 23023-37-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23023-37-2 HCPLUS

CN 1-Isoquinolinamine, 3-(4,5-dimethoxy-2-methylphenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 227 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:115026 HCPLUS

DOCUMENT NUMBER: 70:115026

ORIGINAL REFERENCE NO.: 70:21475a,21478a

TITLE: Isoquinoline imides

INVENTOR(S): Korosi, Jeno; Lang, Tibor; Komlos, Endre; Lujza, Erdelyi

PATENT ASSIGNEE(S): Gyogyszerkutato Intezet

SOURCE: Hung., 11 pp.

CODEN: HUXXAT

DOCUMENT TYPE: Patent

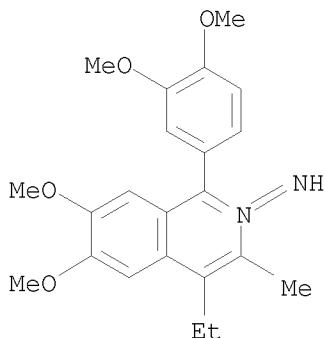
LANGUAGE: Hungarian

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

STN

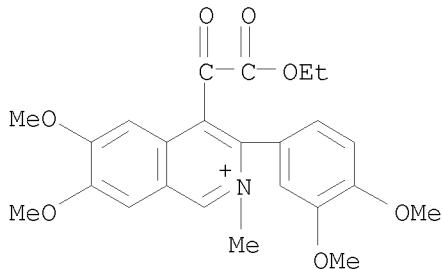
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 155572		19690125	HU	19661209 <--
AB	A mixture of 0.1 mole 3,4,3',4'-tetramethoxy-6-(α -acetopropyl)benzophenone (I), 0.3 mole 100% N ₂ H ₄ .H ₂ O, and 200 ml. absolute EtOH refluxed 3 hrs. and kept overnight deposited 62% 1-hydrazino-1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxy-1H-2-benzopyran, m. 136° (EtOH). A mixture of 0.1 mole I, 0.11 mole 100% N ₂ H ₄ .H ₂ O, and 500 ml. absolute EtOH refluxed 5 hrs., diluted with 100 ml. C ₆ H ₆ , the mixture heated slowly to distil 400 ml. solvent mixture in 3 hrs., and cooled 8 hrs. deposited 19 g. 1-(3,4-dimethoxyphenyl)-4-methyl-5-ethyl-7,8-dimethoxy-5H-2,3-benzodiazepine, m. 136° (EtOH). Either of these 2 compds., or a mixture of them (0.01 mole) was dissolved in 20 ml. MeOH saturated with HCl, the solution evaporated almost to dryness and treated with 20 ml. 5% NaOH to deposit 71% 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisoquinoline-N-imide monohydrate, m. 156-7°, HCl salt m. 217.5° (decomposition), picrate m. 204° (decomposition). The same product was also obtained from 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-di-methoxyisobenzopyrylum chloride with N ₂ H ₄ .H ₂ O and 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisoquinoline with hydroxylamine-O-sulfonic acid.			
IT	22345-48-8P		RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)	
RN	22345-48-8	HCAPLUS		
CN	Isoquinoline, 1-(3,4-dimethoxyphenyl)-4-ethyl-2-imino-6,7-dimethoxy-3-methyl- (CA INDEX NAME)			



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

L13 ANSWER 228 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:28799 HCAPLUS
DOCUMENT NUMBER: 70:28799
ORIGINAL REFERENCE NO.: 70:5381a,5384a
TITLE: 1,2-Dihydroisoquinolines. IX. Acylation. 2
AUTHOR(S): Dyke, Stanley F.; Sainsbury, Malcolm; Brown, David
Whitson; Palfreyman, M. N.; Tiley, E. P.
CORPORATE SOURCE: Bath Univ. Technol., Bath, UK

SOURCE: Tetrahedron (1968), 24(23), 3703-17
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 70:28799
 GI For diagram(s), see printed CA Issue.
 AB The reaction between 1,2-dihydroisoquinolines and a variety of acid chlorides is described, and some properties of the resulting 4-acyl-1,2-dihydroisoquinolines (I) are reported.
 IT 21158-66-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 21158-66-7 HCPLUS
 CN Isoquinolinium, 3-(3,4-dimethoxyphenyl)-4-(2-ethoxy-2-oxoacetyl)-6,7-dimethoxy-2-methyl-, iodide (1:1) (CA INDEX NAME)



● I-

L13 ANSWER 229 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1968:496421 HCPLUS
 DOCUMENT NUMBER: 69:96421
 ORIGINAL REFERENCE NO.: 69:18031a,18034a
 TITLE: Reactions of benzylcarbonyl compounds with formamide.
 I. A novel synthesis of isoquinolines
 AUTHOR(S): Koyama, Takaji; Hirota, Takashi; Ito, Itsuya; Toda, Mutsuko; Yamato, Masatoshi
 CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Kumamoto, Kumamoto City, Japan
 SOURCE: Tetrahedron Letters (1968), (44), 4631-4
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 69:96421
 GI For diagram(s), see printed CA Issue.
 AB Treatment of I ($R = p\text{-MeOC}_6\text{H}_4\text{CH}_2\text{CH}_2$) (II) with hot HCONH_2 and POCl_3 gave a 3:1 mixture of III ($R = p\text{-MeOC}_6\text{H}_4\text{CH}_2\text{CH}_2$) (IV) and III ($R = \text{H}$) (V). IV m. $150\text{--}1.5^\circ$ (MeOH); V m. $201\text{--}2.5^\circ$ (4:1 MeOH-H₂O). Similarly, treatment of I ($R = \text{H}$, Me, Et, and Ph) gave V and the corresponding isoquinolines: 35% III ($R = \text{Me}$), m. $216\text{--}17^\circ$ (MeOH); 30% III ($R = \text{Et}$), m. 177° (MeOH); and 26% III ($R = \text{Ph}$), m. $193.5\text{--}4.5^\circ$ (MeOH). Treatment of I ($R = \text{Ph}$) also gave 2% of a secondary product (VI),

STN

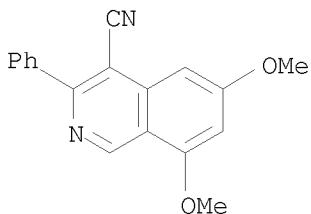
m. 124.5° (C₆H₆-C₆H₁₂) with structure assigned from ir and N.M.R.
data.

IT 19713-14-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19713-14-5 HCAPLUS

CN 4-Isoquinolinecarbonitrile, 6,8-dimethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 230 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:94351 HCAPLUS

DOCUMENT NUMBER: 68:94351

ORIGINAL REFERENCE NO.: 68:18171a,18174a

TITLE: Antitumor activity of isoquinoline derivatives. I.
Relation between chemical constitution and antitumor
(HeLa and Ehrlich) activity

AUTHOR(S): Arai, Yoshihisa; Enomoto, Kingo

CORPORATE SOURCE: Tanabe Seiyaku Co., Osaka, Japan

SOURCE: Yakugaku Zasshi (1968), 88(1), 44-54

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB The isoquinoline compds. were classified into 5 types:

1-unsubstituted-isoquinolines, 1-alkylisoquinolines, 1-arylisoquinolines,
1-aralkylisoquinolines, and bis(isoquinolines). And their in vitro
activity against HeLa cells and in vivo activity against Ehrlich ascites
carcinoma were tested. A parallelism was found between the in vitro and
in vivo activities and the alkyl type compds., especially the ones with
tertiary

alkyl or cycloalkyl group in the 1 position showed a marked inhibitory
effect, while the other 4 types were only slightly active. These data
suggested that the antitumor activity of isoquinoline derivs. was mainly
determined by the chemical structure of the substituent at the 1-position and
in

the alkyl type compds., the activity increased as the number of C atoms in
the alkyl group increased.

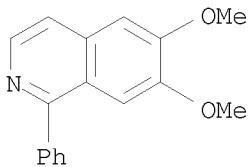
IT 4029-09-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); BIOL (Biological study)
(neoplasm inhibiting activity of)

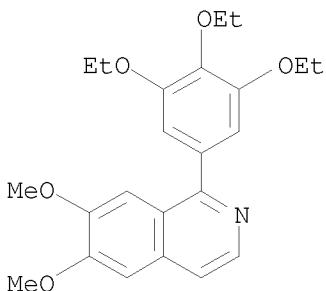
RN 4029-09-8 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)

STN



L13 ANSWER 231 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1967:494034 HCPLUS
DOCUMENT NUMBER: 67:94034
ORIGINAL REFERENCE NO.: 67:17727a,17730a
TITLE: Gas-liquid chromatography of submicrogram amounts of drugs. III. Analysis of alkaloids in biological media
AUTHOR(S): Street, Harold V.
CORPORATE SOURCE: Dep. Forensic Med.Univ. Edinburgh, Edinburgh, UK
SOURCE: Journal of Chromatography (1967), 29(1), 68-79
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. ibid. 23, 232(1966); CA 65: 3668d. Submicrogram amts. of alkaloids were separated by gas chromatog., using a 6 ft. + 0.085 in. stainless steel column packed with 13% SE-30 on 100-120 mesh Chromosorb W. The packing was pretreated by heating in a N stream at 370° for 1.5 hrs. O-free N was the carrier at 50-60 ml./min., and a flame ionization detector was used. The retention times for 29 alkaloids at 10 column temps. are given.
IT 549-68-8
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of)
RN 549-68-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 232 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1967:464223 HCPLUS
DOCUMENT NUMBER: 67:64223
ORIGINAL REFERENCE NO.: 67:12078h,12079a
TITLE: Reaction of 1-arylisobenzpyrylium salts with ammonia

AUTHOR(S): Mueller, Alexander; El-Sawy, Mohamed M.; Meszaros, Miomir; Ruff, Ferenc

CORPORATE SOURCE: L. Eotvos Univ., Budapest, Hung.

SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1966), 50(1-4), 387-401

CODEN: ACASA2; ISSN: 0001-5407

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 67:64223

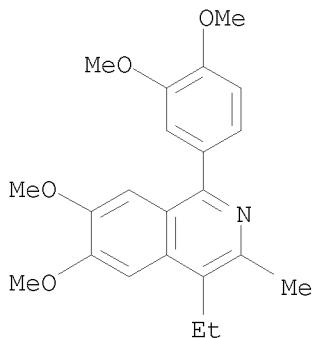
GI For diagram(s), see printed CA Issue.

AB cf. preceding abstract 1-Aryl-2-benzopyrylium salts (I) react with alc. NH₃ under anhydrous conditions to give the 3-hydroxy-3,4-dihydroisoquinoline derivative (II) termed isoquinoline precursors. The hetero ring in II was unstable to alkali, the cleavage of the ring accompanied by loss of NH₃, led to the formation of 2-naphthol derivs. (III). The 3-OH in II is easily split off under acidic conditions to yield the resp. isoquinoline compds. (IV). The possible mechanism of these transformations is discussed. On adding 12 g. I (R = Me, X = HSO₄) (Mueller, et al., CA 49: 15886c) to 300 ml. of a saturated solution of NH₃ in EtOH, decolorization of the salt occurred. After keeping 1 day at 0°, there was collected 7.5 g. II (R = Me) (IIa), m. 157° (Me₂CO). Refluxing a solution of 1 g. IIa in 10 ml. Ac₂O or with 4N HCl yielded IV (R = Me) (IVa), m. 151° (EtOH-ether) [picrate m. 228-9°; ethiodide m. 248°; methosulfate (VI), m. 164°]. The methiodide of IVa, m. 215-16°, reduced by either NaBH₄ or by H over Adam's catalyst, gave V (R = R₁ = Me), m. 54-5° (EtOH). IIa (200 mg.) refluxed with 5 ml. MeI 5 hrs. yielded I (R = Me, X = I), m. 142-3°, which compound on warming with H₂O gave 6-(α -acetylpropyl)-3,3',4,4'-tetramethoxybenzophenone (VII), m. 156° and on NaBH₄ reduction gave 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl-4-ethylisochroman. A mixture of 1 g. IIa, 2.5 ml. Me₂SO₄, 3 ml. H₂O, 2 ml. EtOH, and a solution of 2 g. KOH in 6 ml. H₂O was heated 4 hrs., with Me₃N evolving, then cooled and H₂O added to precipitate 300 mg. III (R = R₁ = Me) (IIIa), m. 145° and 156° (MeOH). Acidification of the alkaline mother liquor yielded III (R = Me, R₁ = H), m. 175°. The same 2 compds. were also obtained by refluxing IIa with 20% NaOH and EtOH, with NH₃ evolving. A solution of 200 mg. IIa, 10 ml. MeOH, 2 drops of H₂O, and 1 g. NaBH₄ was heated, the solvent removed, the sirupy residue dissolved in dilute HCl, and 10% NaOH added to give 120 mg. precipitate of V (R = Me, R₁ = H), m. 60°. Similarly prepared from I (R = H, X = Cl) were: II (R = H) (IIb), m. 214°; III (R = R₁ = H), m. 178-9°, which compound was methylated to IIIa. From IIb and Ac₂O was obtained IV (R = Ac), m. 167° (methiodide m. 190°). IIb treated with HCl yielded IV (R = H) (HCl salt m. 235-6°). IIb treated by H₂O, Me₂SO₄, and KOH gave VII and VI.

IT 1616-49-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and ir and visible spectrum)

RN 1616-49-5 HCPLUS

CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



L13 ANSWER 233 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:464222 HCPLUS

DOCUMENT NUMBER: 67:64222

ORIGINAL REFERENCE NO.: 67:12075a,12078a

TITLE: The reaction of 1-arylisobenzopyrylium salts with ammonia. II

AUTHOR(S): Mueller, Alexander; El-Sawy, Mohamed M.; Meszaros, Miomir; Ruff, Ferenc

CORPORATE SOURCE: L. Eotvos Univ., Budapest, Hung.

SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1967), 52(3), 261-81

CODEN: ACASA2; ISSN: 0001-5407

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. following abstract To 30 g. 1-(3,4-dimethoxyphenyl)-5,6-dimethoxyindan (I) in 1800 ml. HOAc, 20 g. CrO₃ in 40 ml. H₂O and 160 ml. HOAc was added dropwise during 2 hrs. and the mixture was stirred and cooled 1 hr., left 24 hrs. at room temperature, diluted with 1 l. water, and extracted with 3 l.

CHCl₃. The

extract was evaporated, dissolved in 400 ml. HOAc, and treated with 10 ml. 60% HClO₄ on a steam bath 8 min. to give 14 g. II (R = OMe, X = ClO₄), m. 247-8° (HOAc-EtOAc). This product (200 mg.) was dissolved in 50 ml. azeotropic HCl and treated with 300 mg. FeCl₃ in 60 ml. azeotropic HCl to give 210 mg. II (R = OMe, X = FeCl₄), m. 180°. I (9 g.) in 540 ml. HOAc was oxidized with 6 g. CrO₃ and the product was dissolved in 30 ml. HOAc and treated 3 min. with 2 ml. H₂SO₄ to give II (R = OMe, X = HSO₄), m. 235-6°. 1-(3,4-Dimethoxybenzoyl)-3,4-dimethoxyphenylacetal-aldehyde (III) (300 mg.) in 100 ml. EtOAc was treated with 1 ml. 30% HCl, warmed 10 min. on a water bath, and kept overnight at 0° to give 150 mg. II (R = OMe, X = F), m. 245-6°. II (R = OMe, X = ClO₄) (500 mg.) in 15 ml. Me₂CO was refluxed 2.5 hrs. with 2 g. NaOAc.3H₂O in 50 ml. H₂O to give 400 mg. III, m. 167-8°. II (R = OMe, X = HSO₄) (200 mg.) and 10 ml. H₂O was warmed 5 min. on a steam bath to give 120 mg. III. II (R = OMe, X = HSO₄) (2 g.) was added to 50 ml. alc., fractionated with NH₃ at 0°, and the mixture was kept 24 hrs. at 0° to give 1.2 g. 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3,4-dihydro-3-hydroisoquinoline (IV), m. 184° (EtOH). IV (500 mg.) was boiled 2 hrs. in 5 ml. Ac₂O to give 400 mg. 1-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline (V), m.-154° (Me₂CO); picrate m. 168° (HOAc). IV (170 mg.) was

refluxed 5 hrs. with 3 ml. iodine and mixed with 5 ml. ether to give 225 mg. II ($R = OMe$, $X = I$), m. 254-6° (EtOH-ether). The same product was prepared by refluxing a solution of IV in dioxane 3 hrs. with MeI. V (100 mg.) in 2 ml. MeI was refluxed 10 min. to give 140 mg. 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-N-methyl-isoquinolinium iodide (VI), m. 265-6° (Me₂CO), which was quaternized with Me₂SO₄ to give 95% 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-N-ethylisoquinolinium methosulfate, m. 265°. IV (1 g.) was refluxed in 75 ml. MeOH until dissolved, then 2 drops H₂O and 2.5 g. NaBH₄ were added to give 750 mg. 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline, m. 97° (ether). VI (1.2 g.) in 60 ml. MeOH was treated similarly with 3 g. NaBH₄ to give 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-N-methyl-1,2,3,4-tetrahydroisoquinoline, m. 94° (aqueous MeOH). VI could not be hydrogenated over Pd-C. 1-(3,4-Dimethoxyphenyl)- β -(3,4-dimethoxyphenyl)ethylamide (5 g.) and 4.8 ml. POCl₃ in 90 ml. C₆H₆ was refluxed 4 hrs. on a steam bath to give 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3,4-dihydroisoquinoline (VII), m. 165° (Me₂CO); HI salt m. 235° (Me₂CO ether). VII (800 mg.) in 30 ml. C₆H₆ was mixed with 5 ml. MeI and left 4 days at room temperature to give 1 g. 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3,4-dihydro-N-methylisoquinolinium iodide (VIII), m. 242° (3:1 EtOH-ether). VII (700 mg.) was refluxed 4 hrs. with 0.3 ml. Me₂SO₄ and 30 ml. 20% NaOH to give 600 mg. 1-(3,4-dimethoxybenzoyl)-3,4-dimethoxystyrene (IX), m. 115°. VII (1 g.) was treated successively with 1.5 ml. H₂O, 0.5 ml. Me₂SO₄, 1 ml. EtOH, and a cold solution of 1 g. KOH in 2.5 ml. H₂O and the mixture refluxed 3 hrs. to give 600 mg. IX. VII (500 mg.) and 200 mg. 10% Pd-C in 10 ml. xylene was heated to 200° and refluxed 2 hrs. under N to give 400 mg. V. To a Grignard solution of p-anisylmagnesium bromide, prepared from 1.2 g. Mg foil activated with iodine and 6 ml. p-bromoanisole in 80 ml. dry ether, 3.8 g. 5,6-dimethoxyindanone in 50 ml. C₆H₆ was added and the mixture was stirred 3 hrs. at room temperature, mixed

with

10 g. AlCl₃ in 50 ml. ice water for 15 min., and the aqueous phase extracted 3 times with 30 ml. ether. The organic layers were washed, dried, and evaporated to leave an oil that was boiled 1 hr. with 10 ml. Ac₂O and 10 ml. HOAc, poured into H₂O, neutralized, dissolved in 5 ml. alc. and left overnight at 0° to give 1-(4-methoxyphenyl)-6,7-dimethoxy-3H-indene, m. 107° (MeOH). The above product was hydrogenated 6 hrs. at room temperature and pressure with 10% Pd-C to give 1-(4-methoxyphenyl)-6,7-dimethoxyindan, m. 76-7°. This derivative (3 g.) in 168 ml. HOAc was oxidized with CrO₃ as described above and the product was dissolved in 10 ml. HOAc, treated with 1.5 ml. concentrated H₂SO₄, warmed 3 min., and mixed with EtOAc to precipitate 850 mg. II ($R = H$, $X = HSO_4^-$) (X), m. 267-8° (absolute MeOH-ether). X (500 mg.) was left 2 days at room temperature in 20 ml. saturated alc. NH₃ to give 350 mg. 1-(p-methoxyphenyl)-6,7-dimethoxy-3,4-dihydro-3-hydroxyisoquinoline, m. 168° (Me₂CO). β -(3,4-Dimethoxyphenyl)ethylamine (14.2 g.) and 239 g. K₂CO₃ was refluxed in 60 ml. Me₂CO and 18.874 g. freshly prepared p-methoxybenzoyl chloride was added to give 18.4 g. 1-(4-methoxyphenyl)- β -(3,4-dimethoxyphenyl)-ethylamine, m. 124° (CCl₄). Dehydrogenation of 1-(4-methoxyphenyl)-6,7-dimethoxy-3,4-dihydroisoquinoline (XI) with 10% Pd-C under N gave 81% 1-(4-methoxyphenyl)-6,7-dimethoxyisoquinoline, m. 136-70; picrate m. 195° (HOAc). XI (0.594 g.) was refluxed with 0.3 ml. Me₂SO₄ and 6 g. NaOH to give 480 mg. 1-(4-methoxybenzoyl)-3,4-dimethoxystyrene, m. 115°. To a refluxing

solution of 19.49 g. propioveratrone and 7.8 g. iodineactivated Zn foil in 100 ml. C6H6, 20.4 g. Et α -bromoacetate was added dropwise until a reflux reaction began. Heating was then discontinued and the ester was added slowly to allow 1 hr. gentle reflux. After refluxing an addnl. 30 min., the mixture was cooled to give the hydroxy ester, which was refluxed 2 hrs. in 50 ml. dry xylene with freshed dehydrated KHSO4 to give 20 g. Et β -ethyl-3,4-dimethoxycinnamate, b35 200-10°. This ester (21 g.) in 400 ml. alc. was hydrogenated at room temperature and pressure to give

20

g. Et β -ethyl-3,4-dimethoxydihydrocinnamate, b14 195°. This saturated ester (5 g.) was refluxed 4 hrs. with 2 g. NaOH in 28 ml. 50% EtOH to give 3.68 g. β -(3,4-dimethoxyphenyl)- β -ethylpropionic acid, m. 48° (aqueous MeOH). This acid was cyclized with PC15-SnCl4 to yield 87.8% 3-ethyl-5,6-dimethoxy-1-indanone (XII), m. 165° (MeOH); oxime m. 144° (EtOH); 2,4-dinitrophenylhydrazone m. 255-7°. The Grignard reaction with XII as described above gave 69.6% 1-(4-methoxyphenyl)-5,6-dimethoxy-3-ethyl-3H-indene (XIII); m. 78-9° (aqueous MeOH). XIII (5 g.) was hydrogenated at room temperature and pressure with 10% Pd-C to give 4.69 g. 1-(4-methoxyphenyl)-5,6-dimethoxy-3-ethylindan (XIV), b10 210°. XIII or XIV was dissolved in HOAc and oxidized with CrO3 as described above to give 1-(4-methoxyphenyl)-6,7-dimethoxy-1-ethylisobenzopyrylium hydrogen sulfate (XV), m. 210-11° (EtOH-ether). XV (500 g.) in 30 ml. saturated alc. NH3 was left 2 days at room temperature and the product was dissolved in 7 ml. alc. and mixed with an equal volume of a saturated alc. solution

of picrate acid to give 1-(p-methoxyphenyl)-6,7-dimethoxy-3-hydroxy-3,4-dihydro-4-ethylisoquinoline (XVI), m. 223° (EtOAc). XVI was refluxed 2 hrs. with Ac2O, the solvent was evaporated, and the residual oil was mixed with H2O and the crystalline product that formed was dissolved in alc. and mixed with saturated picric acid in alc. at room temperature to give

71.4%

1-(4-methoxyphenyl)-6,7-dimethoxy-4-ethylisoquinoline, m. 216-17°. This base was refluxed with MeI 1 hr. on a water bath and the colorless oil that resulted was mixed with EtOAc to give 92.8% 1-(4-methoxyphenyl)-6,7-dimethoxy-4-ethyl-N-methylisoquinolinium iodide, m. 260° (EtOAc-ether).

IT

47338-66-9P

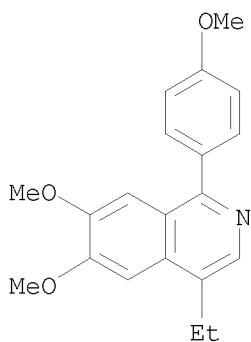
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(The reaction of 1-arylisobenzopyrylium salts with ammonia. II)

RN

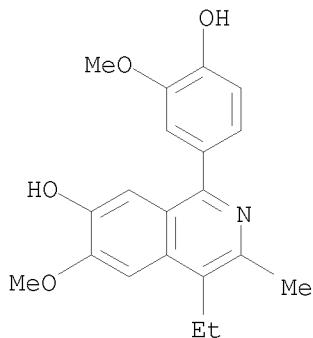
47338-66-9 HCPLUS

CN

Isoquinoline, 4-ethyl-6,7-dimethoxy-1-(4-methoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 234 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1967:115541 HCAPLUS
 DOCUMENT NUMBER: 66:115541
 ORIGINAL REFERENCE NO.: 66:21463a,21466a
 TITLE: 1,5-Diketones. I. Preparation and some reactions of 1-(3-methoxy-4-hydroxyphenyl)-3-methyl-4-ethyl-6-methoxy-7-hydroxyisobenzopyrylium formate, the first isobenzopyrylium salt of an organic acid
 AUTHOR(S): Lempert-Sreter, Magda
 CORPORATE SOURCE: Eotvos Univ., Budapest, Hung.
 SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1966), 50(1-4), 381-6
 CODEN: ACASA2; ISSN: 0001-5407
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB The title compound (I) is prepared in 26% yield. 2 - (1 - Acetylpropyl)-5,4'-diacetoxy-4,3'-dimethoxybenzophenone (II) (Mueller and Horvath, CA 38, 29519) (2 g.) and 4 ml. 85% HCO₂H were refluxed for 4 hrs. The HCO₂H was removed in vacuo to give I, red plates, m. 153-4° (HCO₂H-ether); perchlorate m. 210-13° (AcOH). On prolonged heating with HCO₂H II undergoes transformation. Corresponding formates from IIIa-d are formed on heating with HCO₂H, as shown by their uv spectra, but can not be isolated in the pure state. The aqueous solution of I does not change on standing for 24 hrs.; after 2 days (λ_{maximum} 225, 267 m μ) gradually appears; after approx. 5 days, the spectrum of IVa solution becomes identical with that of II. On heating the aqueous solution, the decomposition takes place in 2 hrs.; in alc. solution it is still faster. I is partially soluble in cold MeOH; on standing, the color of the MeOH solution changes and IVb (cream-colored needles, no sharp m.p., turns deep claret between 110° and 130°) is formed in 88% yield. The alc. solution of IVb on acidification turns yellow. Addition of alkali to I or IVb transforms them through an unstable violet intermediate into II. On treatment with 15% alc. NH₃ at room temperature 48 hrs., I affords 1-(3-methoxy-4-hydroxyphenyl)-3 - methyl - 4 - ethyl - 6 - methoxy - 7 - hydroxyisoquinoline (V) (lemon yellow, m. 213-14°; HCl salt greenish yellow needles, m. 225°) in 80% yield. I and concentrated NH₄OH give 65% 1-(3-methoxy-4-hydroxyphenyl)-3,7-dihydroxy-4-ethyl-3-methyl-6-methoxy-3,4-dihydroisoquinoline (VI), m. 205-10° (aqueous HCONMe₂); HCl salt, m. 210-12° (alc.). I and 15% NH₄OH at 0° 24 hrs. forms 46% V and 40% VI.
 IT 14073-37-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 14073-37-1 HCAPLUS
 CN 7-Isoquinolinol, 4-ethyl-1-(4-hydroxy-3-methoxyphenyl)-6-methoxy-3-methyl- (CA INDEX NAME)



L13 ANSWER 235 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:104058 HCAPLUS

DOCUMENT NUMBER: 64:104058

ORIGINAL REFERENCE NO.: 64:19553h,19554a-h,19555a

TITLE: Reaction of tertiary
6,7-dimethoxy-1,2-dihydroisoquinolines with dilute
acids

AUTHOR(S): Knabe, J.; Ruppenthal, V.

CORPORATE SOURCE: Tech. Hochsch., Brunswick, Germany

SOURCE: Archiv der Pharmazie und Berichte der Deutschen
Pharmazeutischen Gesellschaft (1966),
299(2), 159-65

CODEN: APBDAJ; ISSN: 0376-0367

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 64:104058

GI For diagram(s), see printed CA Issue.

AB cf. CA 61, 4407e. The behavior of the 1,2-dihydroisoquinolines (I-V)
toward dilute acids was investigated.

6,7-Dimethoxy-2-methyl-1-benzyl-1,2-dihydroisoquinolines (I) (and certain
analogs with ether groups on the benzyl ring), rearranged with dilute acids
into the 3,4-dihydroisoquinolinium salt VI, in which the original C-1
substituent shifted to the 3-position. Under the same conditions, II-V
disproportionated into 1-substituted tetrahydroisoquinolines (VII-X) and
the corresponding isoquinolinium salts (XI-XIV). 1-(4'-Bromobenzyl)
analog of I gave products which deviated from scheme 1. XV (9 g.) and 0.3
g. Pd-black in 40 ml. Tetralin boiled 3 hrs. gave 8.3 g. oily XVI; HCl
salt m. 122-4°. From XVII was similarly prepared 80% XVIII, m.
118-20° (Et2O). XIX (18.7 g.) and 0.3 g. Pd-black in 60 ml.
Tetralin boiled 4 hrs. gave 15.8 g. XX, b3 160-5° (bath);
perchlorate m. 132-3° (H2O). XXI and XXII were also prepared from
XXIII and XXIV, resp., by this procedure. XVI, XVIII, XX, XXI, or XXII
treated with MeI in Me2CO-MeOH gave resp. XVI.MeI, m. 196-7°,
205° or 188-90° (the structure of this compound was ensured by
NaBH4 reduction to the corresponding tetrahydroisoquinoline); XI iodide, m.
210-12°; XII iodide, m. 176-7° (decomposition); XIII iodide, m.
248-50°; XIV iodide, whose phys. consts. were identical with XIV
iodide prepared by another route (CA 62, 6458f). Dry powdered XVI.MeI (2.9 g.)
reduced with 2 g. LiAlH4 in Et2O, the solution decomposed with Et2O saturated

with

H2O, the Et2O solution decanted from residue, the residue extracted repeatedly

with Et₂O, the combined Et₂O solns. [containing I, λ (MeOH) 345 m μ] extracted with 3 50-ml. portions 2% HCl, the combined HCl solns. heated 2 hrs. on a water bath [the solution now showed the uv spectrum of VI, λ (MeOH) 255, 320, and 380 m μ], cooled, made alkaline with NaHCO₃, treated with KCN, and extracted with Et₂O, the extract evaporated, the residual oil (1.2 g.; VI pseudocyanide) reduced in MeOH with NaBH₄, the solution worked up, and the base treated in Et₂O solution with HCl gave XXV.HCl, m. 188-9° (Me₂CO-Et₂O), mixed m.p. with 1-benzyl isomer HCl salt (XXVI.HCl), m. 180-1° (Me₂CO-Et₂O), depressed to 173°. XV was converted into XV.MeI, m. 158-60°, which was reduced with NaBH₄ and converted into its HCl salt to give XXVI.HCl. The iodides of XI-XIV reduced sep. with LiAlH₄, and worked up as in the preparation of I, the combined Et₂O solns. [containing II-V, resp.; λ (MeOH) 345-50 m μ] extracted with 2% HCl (with IV and V) or 2% ACOH (with II and III), and the colored extract heated 2-4 hrs. on a water bath until the uv spectrum of the solution corresponded to that of XI-XIV, resp. [λ (MeOH) 255, 292, and 320 m μ], treated with NaHCO₃, and extracted with Et₂O gave VII-X, resp. (for identification see below); the aqueous solns. acidified with HCl and treated with HClO₄ gave the perchlorates of XI-XIV, resp., which were identical (mixed m.p. and uv and ir spectra) with authentic specimens: XI.ClO₄-, m. 212-13° (iso-PrOH-H₂O); XII.ClO₄-, m. 167-8° (MeOH); XIII.ClO₄-, m. 280-1° (iso-PrOH-H₂O); XIV.ClO₄-, m. 175° (EtOH). XVII (0.5 g.) and 0.5 g. MeI dissolved in a little MeOH-Me₂CO and the solution diluted with Et₂O gave 0.7 g. XVII. MeI, m. 188-90°, which reduced in 80% MeOH with NaBH₄ gave VII, m. 74-5° (MeOH-H₂O), which was identical (mixed m.p. and uv and ir spectra) with VII obtained by disproportionation of II. XIX (2 g.) in a little MeOH-Me₂CO treated with 2 g. MeI and the solution diluted dropwise with Et₂O until turbidity gave 1.7 g. XIX.MeI, m. 180-1°, which reduced in MeOH with NaBH₄ gave oily VIII, which treated like XIX, with MeI gave VIII.MeI, m. 197-8°, identical (mixed m.p. and uv and ir spectra) with VIII.MeI obtained after quaternization of VIII obtained by disproportionation of III. XXIII was converted into XXIII.MeI, which reduced with NaBH₄ and quaternized with MeI gave IX.MeI, m. 201-3°, identical (mixed m.p. and uv and ir spectra) with IX.MeI obtained after quaternization of IX obtained by disproportionation of IV. X obtained by disproportionation of V was identical (mixed m.p. and uv and ir spectra) with X prepared by another route (loc. cit.). Pertinent uv data were given.

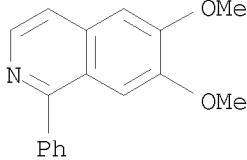
IT 4029-09-8P, Isoquinoline, 6,7-dimethoxy-1-phenyl-

RL: PREP (Preparation)

(preparation of)

RN 4029-09-8 HCPLUS

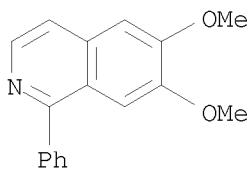
CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

STN

L13 ANSWER 236 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:498174 HCPLUS
DOCUMENT NUMBER: 63:98174
ORIGINAL REFERENCE NO.: 63:18023f-h
TITLE: Dehydrogenation of certain secondary tetrahydroisoquinolines by Hg(II)-EDTA
AUTHOR(S): Knabe, J.; Roloff, H.
CORPORATE SOURCE: Tech. Hochsch., Brunswick, Germany
SOURCE: Archiv der Pharmazie und Berichte der Deutschen Pharmazeutischen Gesellschaft (1965), 298(9), 561-5
CODEN: APBDAJ; ISSN: 0376-0367
DOCUMENT TYPE: Journal
LANGUAGE: German
AB 6,7-Dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinoline (I), m. 112-13°, and 6,7-dimethoxy-1-tert-butyl-1,2,3,4-tetrahydroisoquinoline (II), m. 50-1°, were dehydrogenated by dissolving them in dilute acetic acid, adding Hg(OAc)₂ and EDTA, and heating. Uv examination showed that I yielded a 3,4-dihydroisoquinoline. Chromatography revealed that the products in the reaction mixture consisted of I, 6,7-dimethoxy-1-phenyl-3,4-dihydroisoquinoline and 6,7-dimethoxy-1-phenylisoquinoline, m. 123°, corresponding to 60, 30, and 10% of the starting material. Under similar conditions using II as the starting material, 78% was converted to 6,7-dimethoxy-1-tert-butyl-3,4-dihydroisoquinoline, m. 222-3°, and 7% to 6,7-dimethoxy-1-tert-butylisoquinoline, m. 100-1°. Thus, certain secondary tetrahydroisoquinolines (in which the C-1-substituent cannot be attacked) can be dehydrogenated by Hg(II)-EDTA. The conversion of I is slow, but II is dehydrogenated readily and with good yields.
IT 4029-09-8P, Isoquinoline, 6,7-dimethoxy-1-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 4029-09-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 237 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:462985 HCPLUS
DOCUMENT NUMBER: 63:62985
ORIGINAL REFERENCE NO.: 63:11522a-b
TITLE: Water-soluble salts of isoquinoline bases of the papaverine series
PATENT ASSIGNEE(S): Orgamol S.A.
SOURCE: 5 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable

STN

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
NL 6411317		19650331	NL 1964-11317	19640929 <--
FR 1440625			FR	
GB 1032269			GB	
PRIORITY APPLN. INFO.:			CH	19630930

AB Therapeutically applicable, nonhygroscopic methanesulfonates were prepared. Thus, a solution of 7.3 g. MeSO₃H in 100 ml. AcOEt was dropwise added to a solution of 25.5 g. papaverine in 120 ml. hot EtOH, and the mixture cooled to give 32.5 g. methanesulfonate m. 168-70° (uncor.) with 1:1 solubility in H₂O. The following methanesulfonates were also reported (isoquinoline derivative, m.p. of the salt (uncor.), and solubility in H₂O given):
1-benzyl-3-ethyl-6,7-dimethoxy(eupaverine), 194-6°, 1:1;
1-(β-phenylethyl)-3-ethyl-6,7-dimethoxy, 220-2°, 1:3;
1-(3,4,5-trimethoxyphenyl)-3-methyl-6,7-methylenedioxy-, 208-11°,
1:2; 1-(2-thienyl)-3-ethyl-6,7-dimethoxy-, 213-15°, 1:11;
1-(o-methoxyphenoxyethyl)-3-ethyl-6,7-dimethoxy-, 133.5-5°, 1:7;
1-(phenylthiomethyl)-3-ethyl-6,7-dimethoxy-, 186-8°, 1:6;
1-(α-furyl)-3-ethyl-6,7-dimethoxy-, 170-3°, 1:1.5;
1-(β-pyridyl)-3-ethyl-6,7-dimethoxy-, 197-9°, 1:1.

IT 3962-53-6

RL: PREP (Preparation)

(Derived from data in the 7th Collective Formula Index (1962-1966))

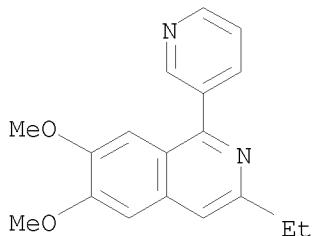
RN 3962-53-6 HCPLUS

CN Isoquinoline, 3-ethyl-6,7-dimethoxy-1-(3-pyridinyl)-, methanesulfonate
(1:1) (CA INDEX NAME)

CM 1

CRN 47206-54-2

CMF C18 H18 N2 O2

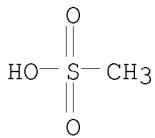


CM 2

CRN 75-75-2

CMF C H4 O3 S

STN



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 238 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:462984 HCAPLUS
DOCUMENT NUMBER: 63:62984
ORIGINAL REFERENCE NO.: 63:11521h,11522a
TITLE: N-Allylnormorphine-6-nicotinic acid ester
INVENTOR(S): Pongratz, Alfred; Zirm, Konrad L.
PATENT ASSIGNEE(S): Lannacher Heilmittel G.m.b.H.
SOURCE: 1 p.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

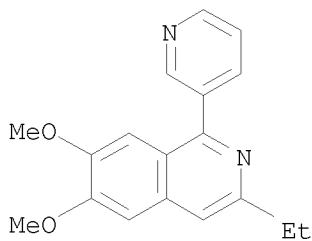
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 241697		19650810	AT	19620907 <--
PRIORITY APPLN. INFO.:			AT	19620907

AB The title compound is made by removing one nicotinic acid residue from N-allylnormorphine-3,6-bis(nicotinic acid ester) or its salts, especially the hydrochloride, either by hydrolysis in aqueous or weakly acidic solution, or by boiling a MeOH solution of the ester in the form of the free base. Preferably, a dilute aqueous solution of the bis(nicotinic acid ester)-HCl is heated to 70-100°, or the solution of the bis(nicotinic acid ester)-HCl in 0.5-1.5N HCl is allowed to stand some days at 10-30° to obtain the N-allylnormorphine-6-nicotinic acid ester, free base m. 180.5-1.5°, hydrochloride m. 200-2°. The compound is characterized by its analgesic activity.

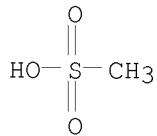
IT 3962-53-6
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 3962-53-6 HCAPLUS
CN Isoquinoline, 3-ethyl-6,7-dimethoxy-1-(3-pyridinyl)-, methanesulfonate
(1:1) (CA INDEX NAME)

CM 1

CRN 47206-54-2
CMF C18 H18 N2 O2



CM 2

CRN 75-75-2
CMF C H4 O3 S

L13 ANSWER 239 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1965:423998 HCPLUS
 DOCUMENT NUMBER: 63:23998
 ORIGINAL REFERENCE NO.: 63:4240e-h, 4241a-d
 TITLE: Preparation of 1-aryl-isobenzopyrylium salts
 AUTHOR(S): Vajda, Miklos
 CORPORATE SOURCE: L. Eotvos Univ., Budapest
 SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1964), 40(3), 295-307
 CODEN: ACASA2; ISSN: 0001-5407
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Various alkyl- and alkoxy-substituted isobenzopyrylium salts (I) were prepared to a mixture of 95 g. propiophenone, 49.5 g. Zn foil (activated with iodine) and 300 ml. anhydrous C6H6 warmed to reflux 101 g. ethyl α -bromopropionate was slowly added (1 hr.) and the mixture refluxed 3 hrs. to give 86 g. II (R1 = R2 = H), b. 152-6°/14 mm. Similarly prepared were the following II (R1, R2, % yield, and b.p./mm. given): MeO, H, 80, 123-5°/0.03; H, MeO, 74, 126-30°/0.03; MeO, MeO, 57, 156-60°/0.02. Heating the appropriate II with about equal weight of KHSO4 at 170-80° for 8 hrs. gave the dehydro compound (III) (R1, R1, and b.p./mm. given): H, H, 150-5°/12; MeO, H, 114-17°/0.03; H, MeO, 150-65°/10; MeO, MeO, 158-70°/0.2. The corresponding saturated acids (IV) were prepared by hydrogenating III in EtOH at atmospheric pressure using 10% Pd-C followed by saponification of the ester by methanolic KOH (R1, R2, b.p./mm. and m.p. given): H, H, 162-5°/10; 118-20°, MeO, H, - 95-7°; H, MeO, 173-5°/12, 78-81°; MeO, MeO, 170-2°/0.01, -. The indanones (V) were

prepared by converting IV to the acid chloride with SOCl_2 in C_6H_6 and effecting the ring closure with AlCl_3 in nitropropane or petr. ether (R1, R2, b.p./mm., and n_{20D} given): H, H, 139-42°/14, 1.5401 (dinitrophenylhydrazone m. 153-5°); MeO, H, 129-30°/0.1, 1.5558; H, MeO, 114-20°/0.01, - (dinitrophenylhydrazone m. 157-9°, semicarbazone m. 159-62°); MeO, MeO, 150-6°/0.03, - (dinitrophenylhydrazone m. 186-7°). The general method for the preparation of 1-arylindenes (VII) involved the addition of

0.075 mole of the appropriate V in 50 ml. anhydrous ether to a solution of 0.15 mole of the appropriate 4-R₃C₆H₄MgBr refluxing the mixture with stirring, pouring into a mixture of ice-H₂SO₄ and working up in the usual way. Thus were prepared VII (R3, R1R2, b.p./mm., and % yield given): H, H, H, 148-52°/0.01, 46; H, MeO, H, 158-61°/0.01, 42; H, H, MeO, 150-8°/0.01, 68; MeO, H, H, 135-45°/0.01, 56; MeO, MeO, H, 168-75°/0.01, 68; MeO, H, MeO, -, - (m. 65-7°); H, MeO, MeO, -, 40 (m. 170-2°). The isobenzopyrylium salts (I) were prepared by oxidation of VII with CrO₃ in AcOH at room temperature and isolation as the perchlorate salt from EtOH or AcOH and ethyl acetate (R1, R2, R3, R4 and m.p. given): H, H, H, H, 143-5°; H, H, H, MeO, 145-7°; H, MeO, H, H, 222-3°; MeO, H, H, H, 206-7°; MeO, H, H, MeO, 198-201°; H, MeO, H, MeO, 172-4°; MeO, MeO, H, H, 195-7°; MeO, MeO, H, MeO, 203-5°; MeO, MeO, (R3R4 =) methylenedioxy, 218-220°; MeO, MeO, MeO, MeO, 209-10°; MeO, EtO, MeO, EtO, 225°; H, H, H, OH, 185-7°; MeO, OH, H, MeO, 205-6°; MeO, OH, MeO, OH, 219-20°.

1-Anisyl-2-methyl-3-ethyl-5-methoxyindane (VIII) was prepared from α-methyl-4-methoxycinnamic acid (X), which was condensed with anisole in the presence of H₂SO₄ to give

β,β-dianisyl-α-methylpropionic acid. This was then cyclized by the Friedel-Crafts method using AlCl₃ to give 1-p-anisyl-2-methyl-5-methoxyindanone (b. 182-90°/0.01 mm., m. 88-9°) which was allowed to react with EtMgBr. The resulting indanol was dehydrated by the action of Ac₂O and a trace of pyridine to give the corresponding indene (m. 73.5-75°) which on hydrogenation gave VIII, also obtained from the corresponding VII. The benzopyrylium salts were converted to isoquinolines (IX) by the action of alc. NH₃ at room temperature or by heating I with a saturated solution of NH₃ in EtOH at 100° for 6 hrs. (R1, R2, R3, R4, and m.p. given): H, MeO, H, H, 142-4°; MeO, H, H, H, 94-5°; MeO, H, H, MeO, 83-4°; MeO, MeO, H, H, 106-7°; MeO, MeO, MeO, MeO, 155-6°. The dissociation consts. of I as determined by polarography and spectrophotometry

are

also given.

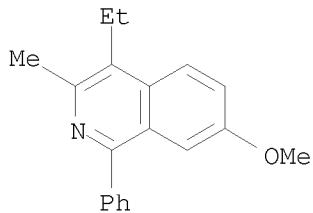
IT 1616-45-1P, Isoquinoline, 4-ethyl-7-methoxy-3-methyl-1-phenyl-
RL: PREP (Preparation)

(preparation of)

RN 1616-45-1 HCPLUS

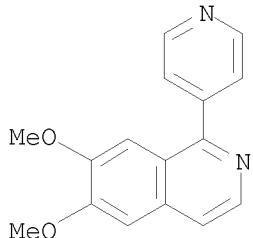
CN Isoquinoline, 4-ethyl-7-methoxy-3-methyl-1-phenyl- (CA INDEX NAME)

STN



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 240 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:93561 HCPLUS
DOCUMENT NUMBER: 62:93561
ORIGINAL REFERENCE NO.: 62:16783g-h
TITLE: Pharmacological activity of some papaverine analogs.
II
AUTHOR(S): Sheikova, Zh.; Nikolova, M
SOURCE: Izvestiya na Instituta po Fiziologiya, Bulgarska Akademiya na Naukite (1964), 7, 243-52
CODEN: IIFBA4; ISSN: 0068-3922
DOCUMENT TYPE: Journal
LANGUAGE: Bulgarian
AB cf. CA 60, 14672h. The spasmolytic activity of the nicotinoyl, isonicotinoyl, and furanoyl derivs. were lower than papaverine (I). The o-methoxyphenol and trimethoxyphenol derivs. had equal or superior spasmolytic effects. The nonhydrated compds. of these derivs. had a depressive effect on the central nervous system, while the hydrated compds. had a stimulant effect. All compds., except those containing furanoyl and o-methoxyphenyl groups were less toxic than I.
IT 3141-78-4, Isoquinoline, 6,7-dimethoxy-1-(4-pyridyl)-(antispasmodic activity of)
RN 3141-78-4 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(4-pyridinyl)-(CA INDEX NAME)



L13 ANSWER 241 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:93560 HCPLUS
DOCUMENT NUMBER: 62:93560
ORIGINAL REFERENCE NO.: 62:16783e-g
TITLE: Relations between chemical structure and pharmacological actions in a series of

STN

AUTHOR(S): γ -lactones and amino alcohols
Zavrazhnov, V. I.; Ponomarev, F. G.; Trukhacheva, L.
I.

CORPORATE SOURCE: Med. Inst., Voronezh
SOURCE: Elektron. i Khim. v Kardiol., Voronezhsk. Obl.
Obshchestvo Kardiologov, Voronezhsk. Obl. Obshchestvo
Terapevtov (1964) 348-58

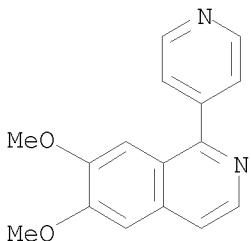
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The effects were investigated of synthetic derivs. of α -aceto- γ -butyrolactone (I), Et acetoacetate, morpholine (II) derivs., and derivs. of diethylaminopropanediol ether (III) on perfused blood vessels of frog's hind limb and of isolated rabbit ear, on rabbit intestinal strips in vitro, and on rabbit blood pressure. The L.D.100 was determined in mice. The introduction of Me and vinyl groups in the β -position or in both β - and γ -positions of I caused a reversal of its pharmacol. properties: the derivs. have a spasmolytic activity on blood vessels without any influence on systemic blood pressure and intestinal smooth muscle. Methylation in the β -position or in both β - and γ -positions enhanced the vasopressor activity of I. The introduction of MeOCH₂, PrOCH₂, and iso-PrOCH₂ groups into I in the γ -position caused an increase of pressor properties; substitution of the propoxy group in the γ -position with Cl decreased the pressor activity of the compound and toxicity but had a neg. influence on intestinal peristaltic movements. Substitution of H. in the NH group of II derivs. by aliphatic groups caused an increase of pressor properties and toxicity. From 7 derivs. of III the most active ones were benzyl and Et derivs. which decreased rabbit blood pressure and caused a constriction of ear and limb blood vessels. All III derivs. inhibited the movements and tonus of the rabbit intestine.

IT 3141-78-4, Isoquinoline, 6,7-dimethoxy-1-(4-pyridyl)-
(antispasmodic activity of)

RN 3141-78-4 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(4-pyridinyl)- (CA INDEX NAME)



L13 ANSWER 242 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1964:466336 HCPLUS
DOCUMENT NUMBER: 61:66336
ORIGINAL REFERENCE NO.: 61:11483h,11484a
TITLE: Infrared spectroscopic investigation of
isobenzopyrylium salts
AUTHOR(S): Vajda, Miklos; Ruff, Ferenc
CORPORATE SOURCE: L. Eotvos Univ., Budapest

STN

SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1964), 40(2), 217-24
CODEN: ACASA2; ISSN: 0001-5407

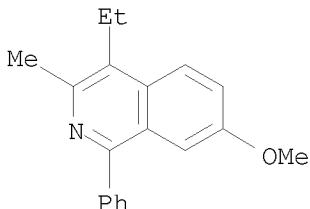
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The infrared spectra of 1-arylisobenzpyrylium salts having various alkyl and alkoxy substituents were investigated and compared with those of analogous isoquinolines. Frequencies for the identification of isobenzpyrylium salts are given and some of them are tentatively assigned to specific vibrations.

IT 1616-45-1, Isoquinoline, 4-ethyl-7-methoxy-3-methyl-1-phenyl- (spectrum of)

RN 1616-45-1 HCAPLUS

CN Isoquinoline, 4-ethyl-7-methoxy-3-methyl-1-phenyl- (CA INDEX NAME)



L13 ANSWER 243 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1964:26272 HCAPLUS

DOCUMENT NUMBER: 60:26272

ORIGINAL REFERENCE NO.: 60:4672h, 4673a

TITLE: Pharmacological effects of some analogs of papaverine
AUTHOR(S): Sheikova, Zh.; Nikolova, M.

SOURCE: Izv. Inst. po Fiziolog., Bulgar. Akad. Nauk. (1963), 6, 253-62

DOCUMENT TYPE: Journal

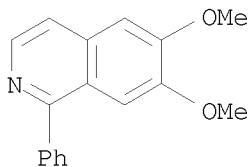
LANGUAGE: Unavailable

AB Eleven analogs of papaverine (I) were evaluated as to their spasmolytic and general effect, and their toxicity. The analogs were: 1-phenyl-, 1-benzyl-, and 1-phenethyl-6,7-dimethoxyisoquinolines, 1-phenyl-, 1-benzyl-, 1-phenethyl-, 1-cinnamoyl-, and 1-isonicotinoyl-6,7-dimethoxydihydroisoquinolines, and 1-phenyl-, 1-benzyl-, and 1-phenethyl-6,7-dimethoxytetrahydroisoquinolines. Only the phenethyl and cinnamoyl substituted compds. showed a slight increase in spasmolytic activity. Substituted compds. with unsatd. bonds in the isoquinoline ring inhibited the central nervous system, produced total atonia, and were less toxic than I. Hydrogenated substitutes excited the central nervous system and were more toxic than I. The isonicotinoyl derivative continuously prolonged the sleep invoked by Na Evipanate.

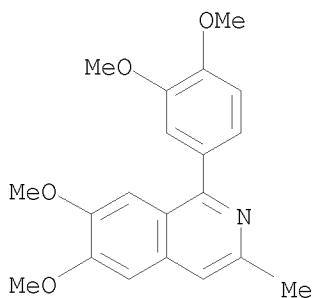
IT 4029-09-8, Isoquinoline, 6,7-dimethoxy-1-phenyl- (pharmacology of)

RN 4029-09-8 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 244 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1963:475483 HCPLUS
 DOCUMENT NUMBER: 59:75483
 ORIGINAL REFERENCE NO.: 59:14036h,14037a-c
 TITLE: Conjugation of a double bond with an aromatic nucleus.
 XXXIII. The synthesis of compounds related to papaverine
 AUTHOR(S): Aparicio, T. Lopez; Lora-Tamayo, M.; Madronero, R.; Marzal, J. Martinez
 SOURCE: Publ. Inst. Quim. "Alonso Barba" (Madrid) (1961), 15, 41-6
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 57, 8496g. Pharmacol. interesting derivs. of 3,4-dihydroisoquinoline were prepared by reaction of isosafrole and O-methylisoeugenol with substituted amides in the presence of POCl₃. A suspension of 0.02 mole of the diene and 0.02 mole of the amide in 10 ml. dry C₆H₆ or PhMe was treated with 5 g. POCl₃ and heated at 90-100° for 1-2 hrs., with exclusion of atmospheric moisture. The product was extracted with ether, precipitated with 20% aqueous NaOH, reextd. with ether, dried over Na₂SO₄, and the ether distilled. The residue was a derivative of 3,4-dihydroisoquinoline. Isosafrole and piperonylamide gave a product m. 124° (picrate, m. 198-9°), consistent with 1-(3,4-methylenedioxyphenyl)-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (I). Isosafrole and β-(p-methoxyphenyl)propionamide gave a product consistent with 1-(p-methoxyphenylethyl)-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline; picrate m. 156-7°. O-Methylisoeugenol and veratramide gave a solid, m. 196-7°, apparently 1-(3,4-dimethoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline. O-Methylisoeugenol and β-(p-methoxyphenyl)propionamide apparently yielded 1-(p-methoxyphenylethyl)-3-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline; picrate m. 139-40°.
 IT 17340-97-5P, Isoquinoline,
 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 17340-97-5 HCPLUS
 CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 245 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:27180 HCAPLUS
DOCUMENT NUMBER: 58:27180
ORIGINAL REFERENCE NO.: 58:4517c-g
TITLE: Derivatives of isoquinoline-5,8-quinone
AUTHOR(S): Lora-Tamayo, Manuel; Madronero, Ramon; Stud, Manfred
CORPORATE SOURCE: Inst. Quim. Alonso Barba, Madrid, Spain
SOURCE: Chemische Berichte (1962), 95, 2176-81
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:27180
AB The demethylation of several 5,8-dimethoxyisoquinoline and 5,8-dimethoxy-1,2,3,4-tetrahydroisoquinoline derivs. yielded the corresponding 5,8-di-OH derivs. which were converted by oxidation to the unstable isoquinoline-5,8-quinones.
1-Methyl-3,4-dihydro-5,8-dimethoxyisoquinoline (0.1 mole) in 20 cc. dry xylene refluxed 4 hrs. with 0.4 g. 10% Pd-C, filtered hot, and cooled gave nearly 100% 1-methyl-5,8-dimethoxyisoquinoline (I); picrate m. 194° (EtOH). Similarly were prepared the 1-Ph and 1-PhCH₂ analogs of I and isolated as the picrates, m. 205 and 215-16°, resp. The appropriate 3,4-dihydroisoquinoline and excess MeI heated 3-5 hrs. with or without Me₂CO or MeCN and cooled gave the corresponding methiodides. In this manner were prepared the following compds. (m.p. given): 1,2-dimethyl-5,8-dimethoxy-3,4-dihydroisoquinolinium iodide (II), 198-9° (EtOH); 1-Ph analog of II, 230° (EtOH); 1-PhCH₂ analog of II, 195-7° (EtOH-Et₂O). The appropriate methiodide (0.005 mole) and 0.01 mole LiAlH₄ refluxed 2 hrs. in Et₂O with stirring and worked up in the usual manner gave the corresponding tetrahydroisoquinolines. In this fashion were prepared the following compds. (m.p. of picrate given): 1,2-dimethyl-5,8-dimethoxy-1,2,3,4-tetrahydroisoquinoline (III), 213° (EtOH); 1-Ph analog of III, 181-3° (EtOH); 1-PhCH₂ analog of III, 160-3° (EtOH). The appropriate 5,8-di-MeO compound (0.01 mole) in 15 cc. HCl heated 2-3 hrs. at 170°, concentrated, and cooled gave the HCl salt of the demethylation product. The appropriate 5,8-di-MeO derivative (0.01 mole) in 50 cc. HBr refluxed 4-5 hrs. and evaporated gave the crystalline HBr salt of the demethylation product; the reaction time can be shortened considerably by heating in a sealed tube or by using HBr of higher concentration By these methods were prepared

the following compds., isolated as the picrates (m.p. of picrate given): 1-methyl-5,8-dihydroxyisoquinoline (IV), 197-9° (EtOH); 1-Ph analog (V) of IV, 215° (EtOH); 1-PhCH₂ analog (VI) of IV, 175-6° (EtOH); 1,2-dimethyl-5,8-dihydroxy-1,2,3,4-tetrahydroisoquinoline (VII), 204° (EtOH); 1-PhCH₂ analog of VII, [HBr salt, m. 220-3° (BuOH.)]. VII.HCl (0.4 g.) in the min. volume H₂O treated with 0.4 g. K₂Cr₂O₇ in 3 cc. H₂O and a few drops concentrated H₂SO₄, cooled to -78°, and filtered, the residue dissolved in Me₂CO, filtered, treated with C, and evaporated, and the crude product dissolved in H₂O and treated with saturated

aqueous picric acid gave the picrate of 1,2-dimethyl-1,2,3,4-tetrahydroisoquinoline-5,8-quinone, m. 164-6°. V.HBr (2 g.) in 100 cc. H₂O treated successively with 100 cc. EtOAc and dropwise with 4.1 g. K₃Fe(CN)₆ and 1.6 g. NaHCO₃ in 100 cc. H₂O at room temperature with stirring and kept overnight, the aqueous layer extracted with EtOAc,

the combined organic layer and extract evaporated, and the oily residue dissolved in

EtOH and treated with saturated aqueous picric acid gave the picrate of 1-phenylisoquinoline-5,8-quinone, m. 194-7° (decomposition). VI gave similarly the picrate of 1-benzylisoquinoline-5,8-quinone, m. 158° (EtOH).

IT 96060-85-4P, Isoquinoline, 5,8-dimethoxy-1-phenyl-, picrate
RL: PREP (Preparation)

(preparation of)

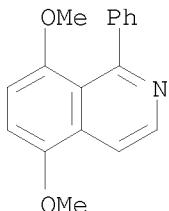
RN 96060-85-4 HCAPLUS

CN Isoquinoline, 5,8-dimethoxy-1-phenyl-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 96060-84-3

CMF C17 H15 N O2

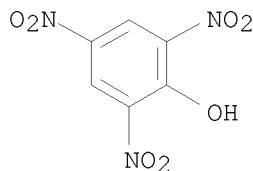


CM 2

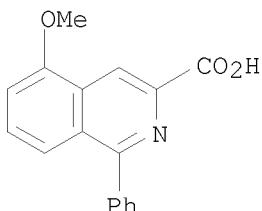
CRN 88-89-1

CMF C6 H3 N3 O7

STN



L13 ANSWER 246 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:436109 HCPLUS
DOCUMENT NUMBER: 57:36109
ORIGINAL REFERENCE NO.: 57:7162h-i
TITLE: Chemistry of lactones. VI. Reaction of unsaturated azlactones under Friedel-Crafts conditions
AUTHOR(S): Filler, Robert; Rao, Y. Shyamsunder
CORPORATE SOURCE: Illinois Inst. of Technol., Chicago
SOURCE: Journal of Organic Chemistry (1962), 27, 2403-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 55, 25906b. The behavior of unsatd. azlactones under Friedel-Crafts conditions has been studied in detail. The course of the reaction is dependent on a variety of factors, including reaction conditions, solvent, and the nature of substituents on the arylidene ring. Four different products have been isolated: saturated azlactones, w-benzamidoacetophenone, 2-benzamidoindenone, and 1-phenylisoquinoline-3-carboxylic acids.
IT 93325-39-4P, 3-Isoquinolinicarboxylic acid, 5-methoxy-1-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 93325-39-4 HCPLUS
CN 3-Isoquinolinicarboxylic acid, 5-methoxy-1-phenyl- (CA INDEX NAME)

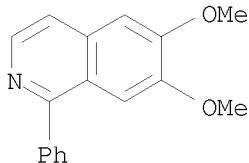


OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 247 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:60554 HCPLUS
DOCUMENT NUMBER: 56:60554
ORIGINAL REFERENCE NO.: 56:11569c-d
TITLE: Synthesis of some simple structural analogs of papaverine
AUTHOR(S): Levy, M.

STN

SOURCE: Farmatsiya (Sofia, Bulgaria) (1961), (No. 4), 25-30
CODEN: FMTYA2; ISSN: 0428-0296
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB By the method previously described (ibid. 1956, Number 1, 20) the following 1-substituted-6,7-dimethoxyisoquinolines, -dihydroisoquinolines, and -tetrahydroisoquinolines were prepared (the substituent and the m.ps for the free bases, maleates, and the HCl salts are given in the above order).
Ph: 112-14°, 119-20°, 124-5°; maleates, 151-3°, 146-7°, 150-3°; HCl salts, 195-6°, 205-6°, -. Benzyl: - (liquid), 99-101°, 95-7°; maleates, 174-6°, 148-9°, 154-6°; HCl salts, 117-20°, 190-1°, -. Phenethyl: 103-5°, 91-2°, 98-100°; maleates, 137-8°, 138-40°, 143-5°; HCl salts, -, -, -. Dehydrogenation of 1-cinnamyl-6,7-dimethoxydihydroisoquinoline-HCl, m. 160-5°, with Raney Ni gave a resinous material and hydrogenation with Pd/C gave 1-phenethyl-6,7-dimethoxydihydroisoquinoline.
IT 4029-09-8P, Isoquinoline, 6,7-dimethoxy-1-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 4029-09-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 248 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:8107 HCPLUS
DOCUMENT NUMBER: 55:8107
ORIGINAL REFERENCE NO.: 55:1612a-h
TITLE: New derivatives of 1-phenylisoquinoline
AUTHOR(S): Delaby, R.; Tsatsas, G.; Jendrot, M. C.
CORPORATE SOURCE: Fac. pharm., Paris
SOURCE: Bulletin de la Societe Chimique de France (1960) 231-9
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:8107
GI For diagram(s), see printed CA Issue.
AB cf. CA 51, 7318e. Substituted 1-phenylisoquinolines (I) were prepared from N-phenethylbenzamides (II) by a Bischler-Napieralski cyclization, followed by dehydrogenation. Phenethyl amines (III), all of which were known, were obtained by hydrogenation of phenylacetonitriles or reduction (Zn.Hg in HCl) of β-nitrostyrenes. Two new benzoic acids were prepared 3-Methoxy-2-propoxybenzaldehyde (40 g.) was oxidized to 33.5 g. 3-methoxy-2-propoxybenzoic acid, m. 49°, by heating it 1 hr. with

60 g. KMnO₄ in 3 l. H₂O. Likewise, 11.6 g. 2-isopropoxy-3-methoxybenzoic acid, m. 46-7°, was prepared from 13.5 g. of the corresponding aldehyde. III and benzoyl chlorides (Schotten-Baumann reaction) gave II. All II distilled at 160-70° under reduced pressure. II were cyclized by POCl₃ in boiling xylene (20 min.). Thus, 1-(2-ethoxy-3-methoxyphenyl)-3,4-dihydro-5,6-dimethoxyisoquinoline was prepared from 12.2 g. N-[2-(2,3-dimethoxyphenyl)ethyl]-2-ethoxy-3-methoxybenzamide. 1-(3,4,5-Triethoxyphenyl)-5,6-dimethoxyisoquinoline was prepared from 5 g. of the corresponding dihydro compound (IV) by refluxing it in 50 ml. Tetralin with 1 g. 10% Pd on pumice stone. Other derivs. were similarly prepared HCl or HBr salts were prepared by passing gaseous HX (X = Cl or Br) into a solution of I or IV in Et₂O. The compds. are to be tested as antispasmodics. The following information was obtained (R1, R2, R3, R4, R5, R6, R7, % yield of II, m.p. of II, % yield of IV, m.p. of IV, IV salt, m.p. of salt, m.p. of I, I salt, m.p. of salt given): MeO, MeO, H, EtO, MeO, H, H, 90, oil, 86-7°, HBr, 157°, 74-5°, HBr, 168-9°; MeO, MeO, H, PrO, MeO, H, H, 100, oil, 89, 94-5°, HCl, 181°, 71-2°, HBr, 154-6°; MeO, MeO, H, iso-ProO, MeO, H, H, 99, oil, 85, 92-3°, HBr, 168-9°, 92-3°, HBr, 195°; MeO, MeO, H, H, (R₅R₆=)OCH₂O, H, 95, 91°, 99, 119-20°, HCl, 195°, 128-9°, HCl, 185-6°; MeO, MeO, H, H, MeO, MeO, H, 86, 97-8°, 89, 136-7°, HBr, 218-20°, 104-5°, HBr, 184-5°; EtO, MeO, H, MeO, MeO, H, H, 99, oil, 90, 84°, HCl, 153-4°, oil, HBr, 140°; EtO, MeO, H, EtO, MeO, H, H, 90, oil, 85, 93-4°, HBr, 164-5°, oil (picrate m. 105°), HBr, 140°; EtO, MeO, H, H, MeO, MeO, H, 100, 99-100°, 94, 86-7°, HBr, 196°, 108°, HCl, 168-9°; PrO, MeO, H, MeO, H, H, 98, oil, 86, 89°, HBr, 160-4°, oil, HBr, 180-1°; PrO, MeO, H, EtO, MeO, H, H, 97, oil, 95, 82-3°, HBr, 192-5°, 59-60°, HBr, 177-8°; H, (R₂R₃=)OCH₂O, MeO, MeO, H, H, 95, 81-2°, 87, 127-8°, HBr, 140-2°, 218-19°, HBr, 150-2°.

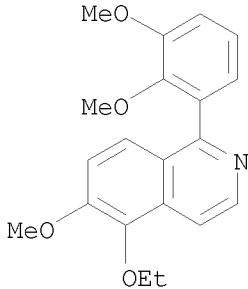
IT 109937-93-1

RL: PREP (Preparation)

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 109937-93-1 HCPLUS

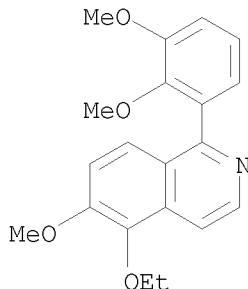
CN Isoquinoline, 1-(2,3-dimethoxyphenyl)-5-ethoxy-6-methoxy- (CA INDEX NAME)



L13 ANSWER 249 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1961:8106 HCPLUS
 DOCUMENT NUMBER: 55:8106

STN

ORIGINAL REFERENCE NO.: 55:1611h-i, 1612a
TITLE: Transformation of basic nitrogenous compounds under destructive hydrogenation. IV. Hydrogenation reactions of 2-picoline and 2-methylquinoline
AUTHOR(S): Yeh, Tsu-Hang; Kalechits, I. V.
SOURCE: Jan Liao Hsueh Pao (1959), 4, 59-68
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 54, 8845e. The destructive hydrogenation of 2-picoline and 2-methylquinoline, catalyzed by iron catalyst, was investigated. The basic nitrogenous compds. obtained were identified. From the product obtained, it was found that deaminocyclization took place under the conditions of destructive hydrogenation. Comparison of the hydrogenation of 2-methylpicoline and 2-methylquinoline indicated that the introduction of a benzene ring increased the reactivity. The hydrogenated product of tetrahydroquinoline was more stable than the product obtained from piperidine. The result indicated that the α -methyl group facilitated hydrogenation of the benzene ring and made it more difficultly demethylated under the exptl. conditions. The structural effect of 2-picoline, quinoline, and 2-methylpicoline on hydrogenation isomerization was also described.
IT 109937-93-1 (Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109937-93-1 HCPLUS
CN Isoquinoline, 1-(2,3-dimethoxyphenyl)-5-ethoxy-6-methoxy- (CA INDEX NAME)



L13 ANSWER 250 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1960:46646 HCPLUS
DOCUMENT NUMBER: 54:46646
ORIGINAL REFERENCE NO.: 54:9204d-e
TITLE: Microchemical identification of atropinelike drugs
AUTHOR(S): Clarke, E. G. C.
SOURCE: Journal of Pharmacy and Pharmacology (1959), 11, 629-36
CODEN: JPPMAB; ISSN: 0022-3573
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The hanging microdrop technique for crystal tests and microdrop reactions on opal glass (C.A. 49, 9880a) were used with 48 atropinelike drugs. Results are tabulated. No clear connection between chemical structure and pharmacol. activity is discernible in the group. The majority of the compds. are esters formed by combination of an amino alc. with a

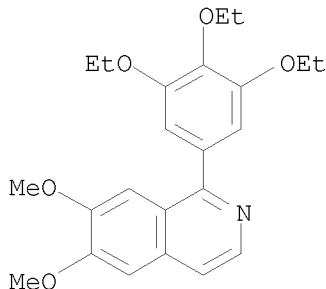
STN

substituted AcOH, but the ester linkage is not essential to the atropinelike activity and both amines and amides with these properties are known.

IT 549-68-8, Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)-
(detection of)

RN 549-68-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 251 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1960:46645 HCPLUS

DOCUMENT NUMBER: 54:46645

ORIGINAL REFERENCE NO.: 54:9204c-d

TITLE: New steroids in therapeutics:

6 α -methylprednisolone

AUTHOR(S): Cueto, Jose L. Pelaez

CORPORATE SOURCE: Univ. Madrid

SOURCE: Revista Clinica Espanola (1959), 75, 189-91

CODEN: RCESA5; ISSN: 0014-2565

DOCUMENT TYPE: Journal

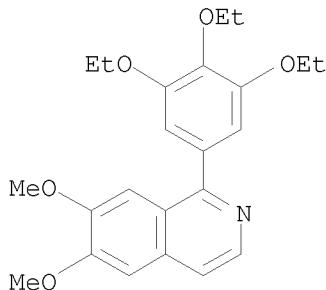
LANGUAGE: Unavailable

AB The pharmacol. of 6 α -methylprednisolone is reviewed. 25 refs.

IT 549-68-8, Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)-
(detection of)

RN 549-68-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 252 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1959:106857 HCPLUS

STN

DOCUMENT NUMBER: 53:106857
ORIGINAL REFERENCE NO.: 53:19172b-d
TITLE: Pharmacology of a new spasmolytic drug
AUTHOR(S): Gyorgy, L.; Borbely, L.; Kertesz, M.; Somkuti, T.; Seress, E.
CORPORATE SOURCE: Med. Univ., Budapest, Hung.
SOURCE: Acta Physiologica Academiae Scientiarum Hungaricae (1959), 15, 189-99
CODEN: APACAB; ISSN: 0001-6756

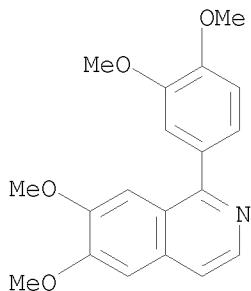
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new papaverine (I) analog is described. 1-(3,4-Dimethoxyphenyl)-6,7-dimethoxy-isoquinoline is given the proprietary name Chinoparine (II). II showed spasmolytic activity identical with that of I, when tested on the coronary flow of the isolated cat heart, excised guinea pig lung, cat intestine in situ, and rat uterus in situ. II decreased blood pressure 30% more than I. Venous pressure was not affected by II, while it was markedly elevated by I. The impairing effect on the cat heart in situ was considerably greater with I than with II. II was less toxic than I in rats: L.D.50 of I and II in rats was 26.25 and 73.33 mg./kg., resp., when administered intravenously and 107.0 and 215.0 mg./kg., resp., when administered intraperitoneally.

IT 15547-50-9, Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (pharmacology of)

RN 15547-50-9 HCPLUS

CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



L13 ANSWER 253 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:61211 HCPLUS
DOCUMENT NUMBER: 52:61211
ORIGINAL REFERENCE NO.: 52:11063a-i
TITLE: The isoquinoline series. II. Synthesis of some 5,6-and 5,8-dimethoxyisoquinolines
AUTHOR(S): Govindachari, T. R.; Lakshmikantham, M. V.
SOURCE: Proceedings - Indian Academy of Sciences, Section A (1957), 46A, 406-15
CODEN: PISAA7; ISSN: 0370-0089
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 50, 8643e. The title compds. were prepared as part of a program on spasmolytic drugs. Condensation of the appropriate BzH with MeNO₂ or EtNO₂ in glacial AcOH containing AcONH₄ gave the following

β -nitrostyrenes (I) $2,3,4,5\text{-RR}_1\text{R}_2(\text{MeO})\text{C}_6\text{HCH:CR}_3\text{NO}_2$ ($\text{R}, \text{R}_1, \text{R}_2, \text{R}_3$, m.p. given): H, H, OMe, Me, $78\text{-}9^\circ$ (dilute AcOH); H, OMe, H, Me, 83° (dilute AcOH); H, H, OMe, H, 120° ; OMe, H, H, H, 88° ; H, OMe, H, H, 108° . I was reduced with LiAlH₄ in the usual manner to give the necessary β -phenylethylamines $2,3,4,5\text{-RR}_1\text{R}_2(\text{MeO})\text{C}_6\text{HCH}_2\text{CHR}_3\text{NH}_2$, (II) ($\text{R}, \text{R}_1, \text{R}_2, \text{R}_3$, b.p./mm., n30D given): H, OMe, H, Me, $147^\circ/4, 1.512$ (HCl salt, m. 147°); H, H, OMe, H, $160^\circ/10, 1.524$; H, H, OMe, Me, $148^\circ/3, -$; OMe, H, H, H, $136\text{-}8^\circ/5, -$; H, OMe, H, H, $143^\circ/3, 1.344$. A mixture of 40 g. $2,3\text{-(MeO)}\text{C}_6\text{H}_3\text{CHO}$, 32 mL. (EtCO)₂O, and 24 g. fused EtCO₂Na was heated 48 h. at 145° and worked up in the usual manner to yield 41 g. $2,3\text{-dimethoxy-}\alpha\text{-cinnamic acid (III)}$, m. 113° (alc.). III (30 g.) was reduced with 5% Na-Hg to yield 28 g. β -(2,3-dimethoxyphenyl)- α -methylpropionic acid (IV), m. 57° (petr. ether). A solution of 44 g. IV, 32 mL. SOCl₂, and 150 mL. dry C₆H₆ was kept at room temperature 24 h. and poured into 700 mL. aqueous NH₄OH containing 10 g. NaOH at 0° to yield 34 g. β -(2,3-dimethoxypenyl)- α -methylpropionamide (V), m. 85° (H₂O). V (7.5 g.) in 30 mL. dioxane was treated with NaOCl in the usual manner to yield 1.5 g. β -(2,3-dimethoxyphenyl)isopropylamine, b. $125^\circ/1$; HCl salt, m. 154° (alc.-Et₂O). II was treated with 95% HCOOH, Ac₂O, BzCl, and PhCH₂COCl to yield β -phenylethylamides $2,3,4,5\text{-R}_1\text{R}_2(\text{MeO})\text{C}_6\text{HCH}_2\text{CHR}_3\text{NHCOR}_4$ (VI) ($\text{R}, \text{R}_1, \text{R}_2, \text{R}_3, \text{R}_4$, m.p. given); H, H, OMe, H, H, 70° ; H, H, OMe, H, Me, $99\text{-}100^\circ$; H, H, OMe, H, Ph, 86° ; H, H, OMe, H, PhCH₂, 105° ; H, H, OMe, Me, H, 78° ; H, H, OMe, Me, $111\text{-}12^\circ$; H, H, OMe, Me, Ph, $155\text{-}6^\circ$; H, H, OMe, Me, PhCH₂, 137° ; OMe, H, H, H, Ph, 86° ; OMe, H, H, H, PhCH₂, 112° ; OMe, H, H, Me, Ph, 70° ; OMe, H, H, Me, PhCH₂, 81° ; H, OMe, H, H, Ph, 115° ; H, OMe, H, H, PhCH₂, 134° ; H, OMe, H, Me, Me, 96° ; H, OMe, H, Me, Ph, 132° ; H, OMe, H, Me, PhCH₂, 120° . The formyl, and Ac derivative of β -(2,3-dimethoxyphenyl)ethyl- and isopropylamines were oils and were cyclized as such. VI was cyclized in dry MePh and POC₁₃ to yield the 3,4-dihydroisoquinolines C(OMe):CR.CH:CR₁.C:C.CH₂.CH.R₂.N:CR₃ (VII) ($\text{R}, \text{R}_1, \text{R}_2, \text{R}_3$, m.p. picrate given): H, OMe, H, H, 160° ; H, OMe, H, Me, 189° ; H, OMe, H, Ph, 195° ; H, OMe, H, PhCH₂, 165° ; H, OMe, Me, H, 203° ; H, OMe, Me, Me, 186° ; H, OMe, Me, Ph, 181° ; H, OMe, Me, PhCH₂, 152° ; OMe, H, H, H, 185° ; OMe, H, H, Me, 234° ; OMe, H, H, Ph, 162° ; OMe, H, H, PhCH₂, 172° ; OMe, H, Me, H, 182° ; OMe, H, Me, Me, 146° ; OMe, H, Me, Ph, 149° ; OMe, H, Me, PhCH₂, 149° . None of the derivs. of β -(2,4-dimethoxyphenyl)ethyl- and iso-Pr amines could be cyclized. VII in Decalin was dehydrogenated with 5% Pd-C to the following isoquinolines: C(OMe):CR.CH:CR₁C:C.CH:C.R₂.N:CR₃ ($\text{R}, \text{R}_1, \text{R}_2, \text{R}_3$, m.p., m.p. picrate given); H, OMe, H, H, $58^\circ, 210^\circ$ (decomposition); H, OMe, H, Me, $54^\circ, 237^\circ$ (decomposition); H, OMe, H, Ph, $124^\circ, 202^\circ$; H, OMe, H, PhCH₂, $89^\circ, 215^\circ$; H, OMe, Me, H, $77^\circ, 243^\circ$ (decomposition); H, OMe, Me, Me, $70^\circ, 230^\circ$; H, OMe, Me, Ph, $118^\circ, 178^\circ$; H, OMe, Me, PhCH₂, $114^\circ, 176^\circ$; OMe, H, H, H, $40^\circ, 211^\circ$; OMe, H, H, Me, $93^\circ, 245^\circ$; OMe, H, H, Ph, $112^\circ, 168^\circ$; OMe, H, H, PhCH₂, $-, 208^\circ$; OMe, H, Me, H, $85^\circ, 241^\circ$; OMe, H, Me, Me, $-, 184^\circ$; OMe, H, Me, Ph, $85^\circ, 180^\circ$; OMe, H, Me, PhCH₂, $134^\circ, 162^\circ$. UV

STN

absorption data are recorded.

IT 114001-53-5

RL: PREP (Preparation)

(Derived from data in the 6th Collective Formula Index (1957-1961))

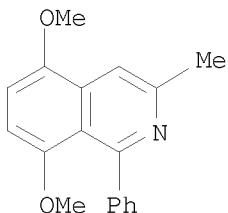
RN 114001-53-5 HCPLUS

CN Isoquinoline, 5,8-dimethoxy-3-methyl-1-phenyl-, compd. with
2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 114001-52-4

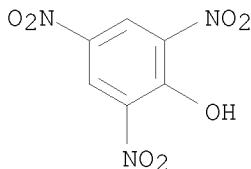
CMF C18 H17 N O2



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L13 ANSWER 254 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1958:50640 HCPLUS

DOCUMENT NUMBER: 52:50640

ORIGINAL REFERENCE NO.: 52:9130c-i, 9131a-i, 9132a-g

TITLE: New aspect of 1-substituted dihydroisoquinolines.
Internal ketimine character. I

AUTHOR(S): Gardent, Jean

CORPORATE SOURCE: Hop. Boucicaut, Paris

SOURCE: Bulletin de la Societe Chimique de France (1957) 1260-70

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB HONH₂ added to most 1-aryl-substituted 3,4-dihydroisoquinolines (I), 1,6,7-RR'2C₉H₆N, at the 1,2-double bond to give pseudooximes (II), 1,6,7,1-RR'2(HOHN)C₉H₅N, converted by the Beckmann rearrangement with P205

to a dihydrocarbostyryl and a primary amine. I EtI compds. (III) also added HONH₂ to give pseudooximes (IV), undergoing the Beckmann rearrangement without cleavage. The dihydropyridine ring of III was opened by BzCl to form Bz derivs. (V, 4,5,2-R'2[EtBzN(CH₂)₂]C₆H₂COR), converted to the oximes (VI). I were prepared by Decker's modification (C.A. 7, 1510) of the Bischler-Napieralski reaction except that 6,7-dimethoxy-3-methyl-1-phenyl-3,4-dihydroisoquinoline (Ia), m. 69-70° (HCl salt, m. 207-8°), was prepared according to the procedure of Kametani (C.A. 47, 10539c). I (R = Ph, R' = EtO) (Ib) (2 g.) heated on a steam bath 30 min. with 2 g. HONH₂.HCl and 5 cc. C₅H₅N and the cooled mixture diluted with H₂O and made alkaline with NH₄OH yielded 90-5% II

(R =

Ph, R' = EtO) (IIb), m. 193°. IIb (2 g.) heated at 100° 1.5 hrs. with 10 cc. HPO₃, diluted with 100 cc. H₂O, made alkaline with NH₄OH, the solution extracted with Et₂O, the extract evaporated, the oily residue taken up in 50

cc. 2% HCl, and the filtered solution made alkaline, filtered from the precipitated Ib,

m. 79° (HCl salt, m. 220°), and the filtrate extracted repeatedly with CHCl₃ yielded 6(7)-ethoxy-7(6)-hydroxy-1-phenyl-3,4-dihydroisoquinoline, m. 190°; HCl salt, m. 233-5°. The alkaline solution from the Et₂O extraction made strongly alkaline with excess KOH, extracted with

CHCl₃, evaporated, the oily residue treated with 5 cc. H₂O and some pellets of KOH, steam-distilled to give PhNH₂, and the cooled distilland extracted twice with CHCl₃ gave 6,7-diethoxy-3,4-dihydroisocarbostyryl, m. 135° (HCl salt, m. 165-70°), identical with a specimen prepared according to Spath and Dobrowsky (C.A. 19, 2959). Ib (4 g.) in a min. of Me₂CO treated with 5 cc. EtI, refrigerated 2 days, and diluted with Et₂O yielded 90-5% Et I salt (IIIb), m. 185-7°. IIIb (2 g.) in H₂O made alkaline with NH₄OH and treated with 2 g. HONH₂.HCl in a min. of H₂O made alkaline with NH₄OH gave 95% pseudooxime (IV, R = Ph, R' = EtO) (IVb), m. 134-5; HCl salt, m. 210-12°. IVb (0.30 g.) treated with 15 cc. 10% HCl and the mixture refluxed 2 hrs. gave HONH₂. IVb (0.50 g.) in 5 cc. HPO₃ heated 1.5 hrs. on a steam bath, the cooled solution diluted with excess H₂O, made alkaline with NH₄OH, extracted with Et₂O, the product converted to the HCl salt,

m. 203-4° (MeOH-Et₂O), and the aqueous solution of the salt made alkaline with NH₄OH gave hydrated 4,5,2-(EtO)₂(EtNHCH₂CH₂)C₆H₂CONHPh, m. 55-60°.

The HCl salt refluxed with 5% alc. KOH, the alc. evaporated, the residue steam-distilled to eliminate PhNH₂, and the distilland extracted with Et₂O yielded 6,7-diethoxy-N-ethyl-3,4-dihydroisocarbostyryl, m. 92°.

IVb in a min. of Me₂CO treated with excess EtI and after 24 hrs. at room

temperature diluted with Et₂O gave IVb EtI salt, m. 180-1°, converted in H₂O by alkalinization with Na₂CO₃ or NaOH to 4,5,2 -

(EtO)₂(Et₂NCH₂CH₂)C₆H₂C(:NOH)Ph, m. 134°, transposed by Beckmann rearrangement to 4,5,2 - (EtO)₂(Et₂NCH₂CH₂)C₆H₂CONHPh, m. 76-7°

(HCl salt, m. 212-13°), saponified by boiling 2 hrs. in 20% KOH in AmOH to the corresponding acid; HCl salt, m. 186-8°. Ib treated

with MeI in Me₂CO and the mixture diluted with Et₂O gave Ib MeI salt, m.

231-3°, giving the corresponding hydroxide, m. 110-11°, by treatment with NaOH, and converted with HONH₂ to the pseudooxime, m. 135°. The pseudooxime stirred 10 min. with excess MeI and the

excess MeI evaporated in vacuo at 0° gave the N-methylpseudooxime MeI salt, m. 170-3° reconverted to the Ib MeI salt by heating in MeOH at 50-60°, to the corresponding hydroxide by heating slowly to

170°, and to the pseudooxime by treatment with aqueous NaOH. Contrary to the N-di-Et series, opening of the piperidine ring in the N-dimethylated series was not possible under the conditions employed. IIIb (0.5 g.) in H₂O made alkaline with NaOH, shaken with 0.30 g. BzCl, and the mixture kept 24 hrs. and filtered gave a quant. yield of V (R = Ph, R' = EtO) (Vb), m. 112-13° (60% alc.); oxime (VI) (R = Ph, R' = EtO) (VIb), m. 173-4° (alc.). Ib (3 g.) in 20 cc. caryophyllene refluxed 15 min. with 3 g. S, the cooled mixture diluted with Et₂O, extracted with

5% HCl, and the acid extract extracted 3 times with CHCl₃ gave 3 g. crude HCl salt, recrystd. from MeOH-Et₂O and converted to the corresponding base, 6,7-dimethoxy-1-phenylisoquinoline, m. 109-10° (alc.); HCl salt, m. 204-7°, unreactive with HONH₂. The above transformations, wholly or in part, were carried out with a series of 1-substituted-3,4-dihydroisoquinolines (Ia-Ih) to give corresponding series of II, III, IV, V, and VI derivs. Ia (2 g.) heated 5 hrs. with 2 g. HONH₂.HCl and 5 cc. C₅H₅N as above gave IIa, m. 191-2°, transposed by heating with HPO₃; the dilute solution basified with KOH, extracted with CHCl₃,

and the product freed from PhNH₂ by steam distillation, taken up in 100 cc. H₂O,

and filtered after 24 hrs. gave 6,7-dimethoxy-3-methyl-3,4-dihydroisocarbostyryl, m. 188°. Ia (3 g.) in 10 cc. C₆H₆ refluxed 7 hrs. with 5 cc. EtI yielded 90% IIIa, converted quantitatively as above to the pseudooxime (IVa), m. about 80°, transposed by Beckmann rearrangement to 4,5,2-(MeO)₂(EtNHCHMeCH₂)C₆H₂CONHPh, m. 129°; HCl salt, m. 221-3°. The anilide (0.25 g.) refluxed 1.5 hrs. in 20 cc.

20% alc. KOH, the alc. evaporated, the residue steam-distilled to give PhNH₂, the

distillate extracted with Et₂O, and the extract washed with 5% HCl and evaporated

gave amorphous 6,7-dimethoxy-N-ethyl-3-methyl-3,4-dihydroisocarbostyryl. IIIa (0.50 g.) in 100 cc. H₂O made alkaline with NaOH, shaken with BzCl, the mixture stored 24 hrs., extracted with Et₂O, the extract washed with H₂O and 5% HCl, evaporated, and the Bz derivative oximated in C₅H₅N with 0.50 g. HONH₂.HCl gave the oxime (VIa), m. 186° (alc.). I (R = 3,4-(MeO)C₆H₃, R' = EtO) (Ic), m. 99-100°, (2 g.) and 3 cc. EtI refluxed 4 hrs. in 5 cc. C₆H₆ yielded 92% IIIc, m. 223-5°, converted quantitatively to IVc, m. 133°, which was benzoylated to Vc, m. 95-7° (C₆H₆-petr. ether); oxime (VIc), m. 180° (alc.). Treatment of 3,4-(EtO)C₆H₃CH₂CH₂NH₂ (VII) with p-O₂NC₆H₄COCl in the presence of NaOH gave 3,4-(EtO)C₆H₃CH₂CH₂NHCOC₆H₄NO₂-p, m. 135°, cyclized by refluxing 1 hr. with an equal weight of POCl₃ in C₆H₆ to 82% I (R = p-O₂NC₆H₄, R' = EtO) (Id), m. 140° (alc.); HCl salt, m. 196-9°. Id treated as above gave IID, m. 188-9° (alc.). Id (1 g.) refluxed 8 hrs. in 5 cc. C₆H₆ with 3 cc. EtI yielded 60% IIId, m. 239-41° benzoylated to Vd, m. 146° (alc.); oxime (VID), m. 143-4° (alc.). VII in C₅H₅N with 3,5-(O₂N)C₆H₃COCl gave the corresponding amide, 3,4-(EtO)C₆H₃CH₂CH₂NHCOC₆H₃(NO₂)₂-3,5, m. 129° (alc.), converted by refluxing 1 hr. in C₆H₆ with an equal weight of POCl₃ to 70% I (R = 3,5-(O₂N)C₆H₃, R' = EtO) (Ie), m. 151-2°; HCl salt, m. 192-5°. Addition of HONH₂ to Ie as above gave the pseudooxime (IIe), m. 212°. I (R = 3,4-(EtO)C₆H₃, R' = EtO) (If) (C.A. 50, 10724b) heated 5 hrs. on a steam bath with HONH₂.HCl in C₅H₅N gave the pseudooxime (IIIf), m. 143-4° (alc.). If shaken with excess EtI in Me₂CO and the mixture diluted with Et₂O gave IIIIf, m.

224-6°, converted to the pseudooxime (IVf), m. 85°.

$\text{Me}(\text{CH}_2)_5\text{CO}_2\text{H}$ (14.8 g.) and 23.8 g. VII refluxed 3 hrs. in 30 cc. xylene with a reflux condenser provided with a Dean and Stark H_2O separator and the cooled solution diluted with 80 cc. petr. ether yielded 90%

3,4-($\text{EtO})_2\text{C}_6\text{H}_3\text{CH}_2\text{CH}_2\text{NHCOCH}_6\text{H}_{13}$, m. 73°, cyclized by refluxing 1 hr.

with POCl_3 in C_6H_6 to 95% I ($\text{R} = \text{C}_6\text{H}_{13}$, $\text{R}' = \text{EtO}$) (Ig), m. 49.5°

(C_6H_6 -petr. ether); HCl salt, m. 147-8°, intensely blue

fluorescence in ultraviolet light. Ig (1.50 g.) refluxed 8 hrs. in 5 cc. C_6H_6 with 3 cc. EtI and the mixture diluted with Et_2O yielded 92% IIIg, m. 150-2°, converted as above to the pseudooxime (IVg), m.

87-9°. IVg (1 g.) in 10 cc. H_3PO_4 , heated 1.5 hrs. on a steam

bath, the diluted solution made alkaline with KOH , extracted with Et_2O , the oily

product refluxed 6 hrs. with 20 cc. 30% alc. KOH , the alc. distilled, the residue steam-distilled, the distillate acidified, concentrated, the concentrate

basified with KOH , and the oil benzoylated gave $\text{C}_6\text{H}_{13}\text{NHBz}$, m.

40-1°. The distilland extracted with Et_2O , the extract washed with H_2O and 5% HCl , the washings set aside, and the Et_2O extract evaporated gave 6,7-diethoxy-N-ethyl-3,4-dihydroisocarbostyryl. The HCl washings extracted with CHCl_3 , made alkaline with KOH , and the oily product benzoylated and crystallized from alc. gave 4,5,2-($\text{EtO})_2(\text{BzEtNCH}_2\text{CH}_2)\text{C}_6\text{H}_2\text{NHBz}$, m.

126-7°. The alkaline solution of saponification after steam distillation and Et_2O extraction

was acidified to give a small amount of $\text{Me}(\text{CH}_2)_5\text{CO}_2\text{H}$. Benzylation of the methiodide IIIg gave a vitreous Bz derivative (Vg) which could not be

oximated. Na (1.20 g.) in 10 cc MeOH treated with 8.36 g. VII and 7.04 g. $\text{PhCH:CHCO}_2\text{Et}$, and the mixture refluxed 1 hr., cooled, and diluted with H_2O yielded 83% 3,4-($\text{EtO})_2\text{C}_6\text{H}_3\text{CH}_2\text{CH}_2\text{NHCOCH:CHPh}$, m. 99° (alc.), which

cyclized by refluxing 1 hr. in C_6H_6 with an equal weight of POCl_3 and the excess POCl_3 destroyed by addition of H_2O gave the HCl salt, m.

172-4°, of I ($\text{R} = \text{HC:CHPh}$, $\text{R}' = \text{EtO}$) (Ih). Ih. HCl (0.40 g.) in 20

cc. H_2O at 0° treated with 0.40 g. HONH_2HCl and 2.50 g. NaOAc in

10 cc. H_2O , the mixture refrigerated 24 hrs., filtered, and the HCl salt, m. about 120°, taken up in very dilute NH_4OH in the presence of Et_2O gave an addition compound, 6,7,1-($\text{EtO})_2[\text{PhCH}(\text{NHOH})\text{CH}_2]\text{C}_9\text{H}_4\text{N}$, m. 100-5°.

The same addition mixture heated 2 hrs. on a steam bath and the oily product extracted with Et_2O yielded PhCH:NOH . The aqueous phase worked up gave

authentic

6,7-diethoxy-1-methyl-3,4-dihydroisoquinoline. Na (0.60 g.) in 5 cc. MeOH refluxed 1 hr. with 4.20 g. VII and 2.95 g. 3-C₅H₄NCO₂Et and the mixture diluted with H_2O gave 3,4-($\text{EtO})_2\text{C}_6\text{H}_3\text{CH}_2\text{CH}_2\text{NHCOCH}_6\text{H}_4\text{N}$, m. 91-2°

(C_6H_6 -petr. ether). The amide (10 g.) refluxed 3 hrs. in PhMe with an equal weight of POCl_3 and the cooled mixture extracted 3 times with H_2O , the aqueous

exts. decanted, basified with KOH , extracted with Et_2O , the exts. treated with C, filtered, extracted with 5% HCl , and the HCl extract extracted with CHCl_3 and

neutralized with KOH yielded 70% I ($\text{R} = 3\text{-C}_5\text{H}_4\text{N}$, $\text{R}' = \text{EtO}$) (Ii), m.

102° (C_6H_6 -petr. ether); HCl salt, prepared by heating an unstable mixture of HCl salts 24 hrs. at 150-60°. Ii was converted to the pseudooxime (IIi), m. 208° (alc.). Ii (1 g.) in 3 cc. C_6H_6 with 2 cc. EtI several days at 0° gave the dimethiodide, m. 195°.

Dehydropapaveraldine, I ($\text{R} = 3,4-(\text{MeO})_2\text{C}_6\text{H}_3\text{CO}$, $\text{R}' = \text{MeO}$) (Ij) (1 g.) refluxed 4 hrs. in 10 cc. C_6H_6 with 2 cc. EtI gave crystalline IIIj, m. 216-18°, soluble in H_2O and giving a precipitate with NH_4OH . IIIj in H_2O

with aqueous 1:1 HONH₂.HCl-NaOAc gave a crystalline HI salt, m. 185-7° soluble in H₂O and converted by basification with NH₄OH to the pseudooxime (IVj), m. 133-4°. Benzylation of IIIJ as above gave Vj, m. 145° (alc.). Cyclization of benzoyltryptamine according to Spath and Lederer (C.A. 24, 2464) gave 1-phenyldihydronorharman (VIII), m. 221-2°.

VIII (0.50 g.) refluxed with 0.50 g. EtI in 10 cc. C₆H₆, the orange gummy EtI addition compound (VIIIa) taken up in H₂O, and the solution treated with 0.50

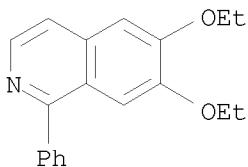
g. HONH₂.HCl in a min. of H₂O and basified with NH₄OH gave the pseudooxime of VIIIa, m. 183°. The combined results demonstrated the unique reactivity of the C-1 atom of 1-substituted 3,4-dihydroisoquinolines.

IT 101890-10-2P, Isoquinoline, 6,7-diethoxy-1-phenyl-, hydrochloride

RL: PREP (Preparation)
(preparation of)

RN 101890-10-2 HCPLUS

CN Isoquinoline, 6,7-diethoxy-1-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 255 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:50634 HCPLUS
DOCUMENT NUMBER: 52:50634
ORIGINAL REFERENCE NO.: 52:9128d-h
TITLE: Synthesis of derivatives of
4-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline
AUTHOR(S): Quelet, Raymond; Mansouri, Mehdi; Pineau, Robert
CORPORATE SOURCE: Fac. Sci., Paris
SOURCE: Compt. rend. (1957), 245, 537-9
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:50634
AB An earlier note (C.A. 50, 8535e) described the condensation of veratrole with aminodiethylacetal to give 1,1-bis-(3,4-dimethoxyphenyl)-2-aminoethane (I) (80% yield) in AcOH in the presence of H₂SO₄. The N-Ac, N-Pr, and N-Bu derivs. (II) of I were obtained when the corresponding N-acylaminoacetals were used in the condensation. Compound I and its N-acyl derivs. were transformed into isoquinolines in order to compare the physiological properties of these products with those of papaverine. Using the method of Pictet and Spengler (C.A. 5, 3423) 5 g. I, 10 cc. MeOH, 5 cc. 40% formalin, and 10 cc. concentrated HCl was mixed and refluxed 2 hrs. giving 70% 6,7-dimethoxy-4-(3,4 - dimethoxyphenyl) - 1,2,3,4 -

tetrahydroisoquinoline (III), m. 147° (MeOH); HCl salt, m. 240°; picrate, m. 233°. An attempt at Pd-catalyzed dehydrogenation of III was unsuccessful. II refluxed with POC₁₃ in toluene (method of Pictet and Finkelstein, C.A. 3, 2435; Ber. 42, 1979(1909), and Decker, and Kropp, C.A. 3, 2455) gave 3,4-dihydro-6,7-dimethoxy-4-(3,4-dimethoxyphenyl)-1-alkyl (or aryl) isoquinolines (IV), yield 60-75%. The following IV were reported (1-substituent, m.p. of base, HCl salt, and picrate given): Me, 70°, 191-2°, 220-1°; Et, 129°, -, 190-1°; Ph, 129-30°, 163-4°, 167-8°. IV were dehydrogenated in 80% yield to the corresponding isoquinolines (V) by Pd in boiling PhMe. The following V were reported (1-substituent, m.p. of base, HCl salt, and picrates given): Me, 207-8°, 211-12°, 240°; Et, 176°, -, 222-3°; Ph, 105-7°, -, 224°.

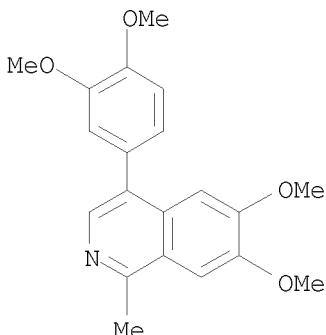
IT 102012-78-2

RL: PREP (Preparation)

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 102012-78-2 HCPLUS

CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L13 ANSWER 256 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1958:50633 HCPLUS

DOCUMENT NUMBER: 52:50633

ORIGINAL REFERENCE NO.: 52:9128b-d

TITLE: Reaction of phenyl- and p-tollyllithium with 1-arylisouinolines

AUTHOR(S): Gilman, Henry; Soddy, Theodore

CORPORATE SOURCE: Iowa State Coll., Ames

SOURCE: Journal of Organic Chemistry (1957), 22, 1716-17

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The addition of aryllithium reagents to 1-arylisouinolines was studied. 1-p-Tolyl- (I) and 1-phenylisouinoline (II) treated with PhLi (III) and

p-MeC₆H₄Li (IV), resp., gave in each case 1-phenyl-p-(1-tolyl)-1,2-dihydroisoquinoline (V). This fact was demonstrated by mixed decomposition point and identical infrared spectra. Both of the spectra contained a 1,4-disubstituted Ph band at 12.3 μ , a Ph ring band at 6.15 μ , and an NH band at 3.1 μ . II (16 g.) in 200 ml anhydrous Et₂O was treated dropwise with 0.08 mole IV in 90 ml. Et₂O; after the addition of 2, 5, and 8 ml. IV solution the reaction became red, brown, and finally dark green in color; the green color was present throughout the remainder of the addition. On completion of the addition the mixture refluxed

45

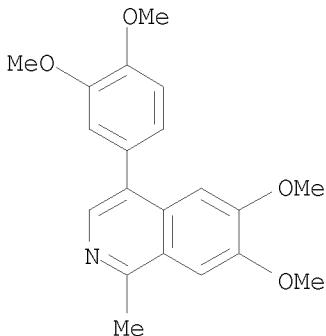
min., hydrolyzed with saturated NH₄Cl, and the Et₂O extract dried, the Et₂O removed, and the residue dissolved in alc., treated with C, filtered, and evaporated gave 0.5 g. V, decompose 176-8°. I (19 g.) in 200 ml. Et₂O treated with 0.09 mole III in 100 ml. Et₂O and the mixture worked up as in the preceding method gave 0.5 g. V.

IT 102012-78-2

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 102012-78-2 HCPLUS

CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L13 ANSWER 257 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1958:40607 HCPLUS

DOCUMENT NUMBER: 52:40607

ORIGINAL REFERENCE NO.: 52:7320a-i, 7321a

TITLE: Cyclic nitrones. II. Polymers of
2,3,4,5-tetrahydropyridine N-oxide and related
compounds

AUTHOR(S): Thesing, Jan; Mayer, Hans

CORPORATE SOURCE: Tech. Hochschule, Darmstadt, Germany

SOURCE: Justus Liebigs Annalen der Chemie (1957),
609, 46-57

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 52:40607

AB cf. C.A. 51, 10516a. N-Hydroxypiperidine (Ia) (0.04 mole) with 0.2 mole KOH in 50 cc. H₂O at 20-5° was treated dropwise with 0.08 mole K₃Fe(CN)₆ in 80 cc. H₂O, diluted with H₂O and kept 2 hrs. at 20° in the dark, cooled to 0° saturated with K₂CO₃, and extracted with CHCl₃ giving 97% (C₅H₉ON)₃ (I) (mol. weight in C₆H₆ 268-318), exploding on attempted distillation in vacuo, pH 8-9 in H₂O. After standing 3 weeks, I gave an orange mass, which in aqueous Me₂CO cooled to -15° yielded 41% (C₅H₉ON)₂ (II), m. 126-7° (described previously, loc. cit.), and unidentified high polymers. I (0.85 g.) within 2 hrs. after preparation was hydrogenated in 75 cc. N HCl with PtO₂ at 20°/760 mm. giving 98.5% (crude yield) Ia.HCl, m. 142-3°. II (0.3 g.) in 20 cc. 2N HCl was added promptly to 40 cc. 20% NaOH at 20°, cooled to 0°, saturated with K₂CO₃, and extracted with CHCl₃ giving I quantitatively. When II in HCl was kept 12 hrs. prior to treatment with NaOH, the mol. weight of the resulting product rose from 297 to 402. To 26.7 g. PhMgBr in 70 cc. absolute Et₂O was added dropwise freshly prepared I in 100 cc. Et₂O and the mixture refluxed 4 hrs. giving a brown oil crystallizing gradually at 20°, which was decomposed with alkaline aqueous NH₄Cl and extracted with Et₂O yielding 2-Ph derivative (III) of Ia, m. 111-12° (petr. ether) (described previously, loc. cit.). III (6.2 g.) in 160 cc. Me₂CO and 16 cc. H₂O was treated within 1-2 min. with 15.2 g. yellow HgO, shaken 1.5 hrs., kept 16 hrs., filtered, and washed with Me₂CO. The evaporated filtrate gave 6.13 g. oil which after 6 days at 0° triturated with little AcOEt gave 1.76 g. colorless dimer (IV) of the 2,3,4,5-tetrahydro-2-phenylpyridine N-oxide, C₂₂H₂₆O₂N₂, m. 200-1° (decomposition) (iso-Am20); the m.p. varies with rate of heating. In weakly alkaline solution IV gradually gave a pink color with triphenyltetrazolium chloride (V). IV (0.4 g.) in hot iso-Am20 with 0.8 g. PhMgBr in 10 cc. Et₂O was refluxed and stirred at 110-20°, cooled, decomposed with NH₄Cl in dilute NH₄OH, and extracted with Et₂O giving 0.56 g. oil, which triturated with MeOH gave 0.21 g. 6-Ph derivative (VI) of III, m. 165-6° (EtOH), giving an immediate red color with V. VI (0.25 g.) in 25 cc. warm H₂O and 6 cc. HCl heated 3 hrs. at 100° with Zn dust, cooled, and made alkaline with concentrated NaOH gave 0.22 g. crude iso-2,6-diphenylpiperidine, identified as the HCl salt, m. 224-5°; HBr salt, m. 258-9°, and HI salt, m. 256-7° (cf. Gilman and Edward, C.A. 48, 3974f), identical with those prepared from 2,6-diphenylpyridine reduced with EtOH and Na. To 16.8 g. 1,2,3,4-tetrahydroisoquinoline (VII) was added dropwise 12.8 g. CH₂:CHCO₂Et and the mixture heated 1 hr. at about 90-100° giving 24.25 g. N-carbethoxyethyl-1,2,3,4-tetrahydroisoquinoline (VIII), b15 188-9°. To 12 g. VIII in 100 cc. absolute Et₂O at 0-5° was added 180 cc. Et₂O containing o-HO₂CC₆H₄CO₃H [Organic Syntheses, Collective Volume III, 619(1955)] giving a viscous oil from which the Et₂O solution (IX) was decanted. The oil in 100 cc. 2N NaOH saturated with K₂CO₃ was heated 1 hr. at 80-90°, diluted with 100 cc. H₂O, and extracted with Et₂O (including extract IX) giving 37-45% crude 2-hydroxy-1,2,3,4-tetrahydroisoquinoline (X), purified through its HCl salt, m. 153-4° (Me₂CO); this with aqueous NaOH gave X, m. 80-1° (cyclohexane), giving an immediate red color with V [picrate of X, m. 143-4° (H₂O)]. Crude X decomposed rapidly in a desiccator; pure X proved quite stable. X, prepared from VII in aqueous Me₂CO with H₂O₂, was obtained in only 2% yield [cf. Maass and Wolffenstein, Ber. 30, 2189(1897)]

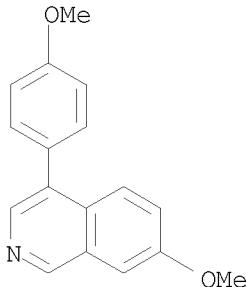
and 31, 2687(1898) who termed X "o-aminomethylphenylacetaldehyde" (m. 76-7°)]. X (0.48 g.) in 15 cc. Me₂CO and 1.5 cc. H₂O was shaken 1.5 hrs. with 1.4 g. HgO; the evaporated filtrate gave the crude nitrone, 3,4-dihydroisoquinoline N-oxide (XI), purified through the picrate, m. 142.5-3.5° (MeOH), 0.84 g. of which was warmed at 50° with 18% HCl, extracted with PhNO₂ and Et₂O, and the aqueous phase poured into 40 cc. 2N NaOH at 0° over a layer of CHCl₃, saturated with K₂CO₃, and well shaken. The CHCl₃ extract gave 0.3 g. hygroscopic XI, m. 56-7° (after evaporation, keeping 14 days at 0°, triturating with absolute Et₂O, and drying over P₂O₅). XI gave no color with V. The marked differences in the HgO dehydrogenations of III and X are discussed fully and explained on the basis of configurational analyses. Ultraviolet spectra of XI and of benzaldehyde N-methylnitrone and the infrared spectrum of IV are given and discussed. 27 references.

IT 101442-06-2

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 101442-06-2 HCPLUS

CN Isoquinoline, 7-methoxy-4-(4-methoxyphenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

L13 ANSWER 258 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1958:40606 HCPLUS

DOCUMENT NUMBER: 52:40606

ORIGINAL REFERENCE NO.: 52:7319h-i,7320a

TITLE: Syntheses of isoquinoline derivatives of pharmacological interest

AUTHOR(S): Deshpande, V. N.; Nargund, K. S.

CORPORATE SOURCE: Karnatak Univ., Dharwar, India

SOURCE: Journal of the Karnatak University (1956), 1, 15-18

CODEN: JKAUAR; ISSN: 0453-3348

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The β,β-diarylsubstituted ethylamine (0.005 mole) was treated with 40% formalin (slight excess over 0.008 mole). The intermediate Schiff bases were obtained as pastes and were cyclized by the action of 24% HCl. Isoquinoline bases thus formed were characterized by the formation of picrates. The bases (0.250 g.) were dehydrogenated by 10% Pd-C by heating the mixture at 210-15° for 15 min. and the resulting isoquinoline derivs. were isolated as the picrate. Below are given compds. and m.ps. of the tetrahydroisoquinoline base, its picrate, and the

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picrate of the isoquinoline base: 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline, 106°, 195°, 269°; 4-(4-methoxyphenyl)-7-methoxy-1,2,3,4-tetrahydroisoquinoline, 92°, 240°, 168°; 4-phenyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline, 173°, 219°, 236°; 4-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline, 76°, 163°, 244°; 4-(2,4-dimethoxyphenyl)-1,2,3,4-tetrahydroisoquinoline, 182°, 230°, 204°.

IT 102593-25-9

RL: PREP (Preparation)

(Derived from data in the 6th Collective Formula Index (1957-1961))

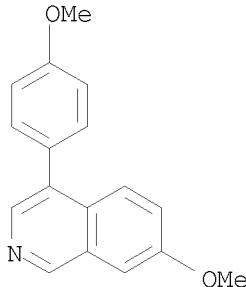
RN 102593-25-9 HCAPLUS

CN Isoquinoline, 7-methoxy-4-(4-methoxyphenyl)-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 101442-06-2

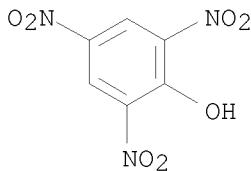
CMF C17 H15 N O2



CM 2

CRN 88-89-1

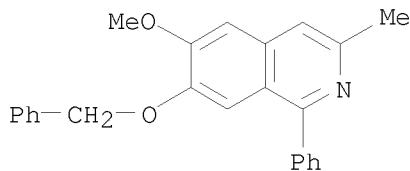
CMF C6 H3 N3 O7



L13 ANSWER 259 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:86480 HCAPLUS
DOCUMENT NUMBER: 51:86480
ORIGINAL REFERENCE NO.: 51:15699h-i,15700a
TITLE: Synthetic compounds active against
Salmonella-dysentery group bacilli
AUTHOR(S): Akiya, Shichiro

STN

CORPORATE SOURCE: Univ. Tokyo
SOURCE: Japanese Journal of Experimental Medicine (1956), 26, 91-112
CODEN: JJEMAG; ISSN: 0021-5031
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Synthetic organic compds. (1028) were tested for their in vitro antibacterial activities against Micrococcus pyogenes var. aureus, Escherichia coli Number 1, Shigella dysenteriae Ewing I, Shigella paradyserteriae 2a, Salmonella typhosa S 57, S. paratyphi A 1015, and S. enteritidis 5168. Of these compds. 436 were effective at 10⁻⁴M against at least one of the organisms. Active compds. comprised hydrazone derivative of 5-nitrofurfural, benzoquinone and naphthoquinone derivs., alkyl and acyl resorcinols, N-containing heteroarom. quaternary bases, aminodibenzofurans, hydrazones of pyridine derivs., aromatic aldehydes, tricarbonylmethane derivs., and others.
IT 102664-48-2, Isoquinoline, 7-(benzyloxy)-6-methoxy-3-methyl-1-phenyl- (bactericidal action of)
RN 102664-48-2 HCPLUS
CN Isoquinoline, 6-methoxy-3-methyl-1-phenyl-7-(phenylmethoxy)- (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

L13 ANSWER 260 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1956:16405 HCPLUS
DOCUMENT NUMBER: 50:16405
ORIGINAL REFERENCE NO.: 50:3445b-e
TITLE: Conjugation between a double bond and an aromatic nucleus. XXIX. Condensation reactions with imidoxy chlorides (use of amides as precursors)
AUTHOR(S): Pelaez, R. Madronero; Alvarez, Eldiberto Fernandez; Tamayo, M. Lora
CORPORATE SOURCE: Univ. Madrid
SOURCE: Anales de la Real Sociedad Espanola de Fisica y Quimica, Serie B: Quimica (1955), 51B, 276-82
CODEN: ARSQAL; ISSN: 0034-088X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 49, 4603e. Derivs. of 3,4-dihydro-6,7-methylenedioxy- and 3,4-dihydro-6,7-di-methoxyisoquinoline HCl salt (I and IA, resp.) are prepared in 30-60% yield by a Diels-Alder addition of imidoxy chlorides [produced from amides and POC13 (II) in the presence of the dienes] to vinyl-substituted aromatic compds. Isoveratrole (III) (0.02 mole), 0.025 mole HCONH2 (IV), 10 cc. PhMe, and 10 cc. II refluxed 1-2 hrs. at

120-30°, cooled, poured into ice water, the excess III and IV extracted with Et₂O, made alkaline with NaOH, extracted with Et₂O, and the Et₂O layers washed with H₂O, dried, and saturated with dry HCl, precipitate the 3-Me derivative, m.

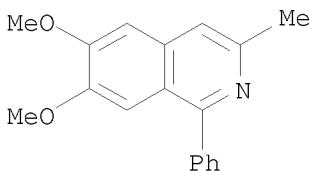
187° of IA. Similarly are prepared the following derivs. of I: 3-Me, from isosafrole (V) and II, m. 198°; 1,3-di-Me, from V and AcNH₂ (VI), m. 220-1°; 1-phenyl-3-methyl, from V and BzNH₂ (VII), m. 206-8°; 1-benzyl-3-methyl, from V and PhCH₂CONH₂ (VIII), m. 184-5°. Derivs. of IA: 1,3-di-Me, from III and VI, m. 216°; 1-phenyl-3-methyl, from III and VII, m. 203-5°; 1-benzyl-3-methyl, from III and VIII, m. 185°. The substituted I and IA are aromatized by heating the free base in PhNO₂ 1 hr. at 200°. Heating PhCN and V at 100° in a stream of dry HCl gave 2,4,6-triphenyl-s-triazine.

IT 879679-66-0P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Conjugation between a double bond and an aromatic nucleus. XXIX. Condensation reactions with imidoyle chlorides (use of amides as precursors))

RN 879679-66-0 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-3-methyl-1-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L13 ANSWER 261 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1955:84276 HCAPLUS

DOCUMENT NUMBER: 49:84276

ORIGINAL REFERENCE NO.: 49:15902h-i,15903a-i

TITLE: Chemistry of vanillin and its derivatives. VI.

Effective spasmolytic 1-phenylisoquinolines and diphenethylamines containing the guaiacyl grouping

Kratzl, K.; Horejschi, T.; Billek, G.

AUTHOR(S): Kratzl, K.; Horejschi, T.; Billek, G.

CORPORATE SOURCE: Univ. Vienna

SOURCE: Monatshefte fuer Chemie (1954), 85, 1154-65

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 49:84276

AB cf. C.A. 48, 1363g. Several 1-phenylisoquinolines were prepared from 4-(2-aminoethyl)guaiacol (I) and its benzyl ether (II), by forming amides, treating these with POCl₃, and dehydrogenating. The following amides were prepared by treatment with the corresponding acyl or alkyl chloride (starting material, yield, and m.p. given): BzNHCH₂CH₂C₆H₃(OH)OMe-4,3, I,

94, 127°; BzNHCH₂CH₂C₆H₃(OBz)OMe-4,3 (III), I, -, -; BzNHCH₂CH₂C₆H₃(OCH₂Ph)OMe-4,3 (IV), I (or II), 76, 134°; 3,4-MeO(AcO)C₆H₃CONHCH₂CH₂C₆H₃(OH)OMe-4,3, I, 89, 117-20°; 3,4-MeO-(BzO)C₆H₃CONHCH₂CH₂C₆H₃(OH)OMe-4,3 (V), I, 95, 133-6°; 3,4-MeO(PhCH₂O)C₆H₃CONHCH₂CH₂C₆H₃(OH)OMe-4,3 (VI), I, 93, 146-7°; 3,4-MeO(BzO)C₆H₃CONHCH₂CH₂C₆H₃(OBz)OMe-4,3, V, 87, 154-5°; 3,4-MeO(PhCH₂O)C₆H₃CONHCH₂CH₂C₆H₃(OBz)OMe-4,3, VI, 90, 143°; 3,4-MeO(PhCH₂O)C₆H₃CONHCH₂CH₂C₆H₃(OCH₂Ph)OMe-4,3 (VII), IV or II, 75-89, 167°; and 3,5,4-(MeO)₂(PhCH₂)OC₆H₃CONHCH₂CH₂C₆H₃(OCH₂Ph)OMe-4,3 (VIII), II, 67, 125°. For the ring-closure, 5 millimoles of the amide was treated with 12.5 millimoles POCl₃ in 60 ml. absolute xylene or PhMe at reflux for 20-60 min. The product was precipitated as a resinous mass by addition of petr. ether. The free base could be precipitated from dilute HCl solution

(containing EtOH if necessary) by NH₃ and recrystd. from EtOH-H₂O. The hydrochloride could be recovered instead by excess concentrated HCl. The picrate was prepared from the free base with picric acid or from the hydrochloride with sodium picrate. In this way were made the following 3,4-dihydroisoquinolines and derivs. (substituents, starting compound, % yield, m.p. given): 7-benzoyloxy-6-methoxy-1-phenyl (IX), III, 78, 191-2° (picrate, m. 210-12°; hydrochloride, m. 209-12°); 7-benzylloxy-6-methoxy-1-phenyl, IV, 88, 137° (hydrochloride, m. 199°); 7-benzylloxy-1-(4-benzylloxy-3-methoxyphenyl)-6-methoxy (X), VII, 79, - (picrate, m. 203°); 7-benzylloxy-1-(4-benzylloxy-3,5-dimethoxyphenyl)-6-methoxy (XI), VIII, 77, - (picrate, m. 232°). Hydrolysis of IX with aqueous EtOH-NaOH gave 93% 6-methoxy-1-phenyl-3,4-dihydro-7-isoquinolinol, m. 180° (picrate, m. 240°; hydrochloride, m. 210-12°). Treatment of X with 20% HCl and recrystn. from dilute HCl gave 93% 1-(4-hydroxy-3-methoxyphenyl)-6-methoxy-3,4-dihydro-7-isoquinolinol hydrochloride (m. 258°). Similarly, XI gave 92% 1-(4-hydroxy-3,5-dimethoxyphenyl)-6-methoxy-3,4-dihydro-7-isoquinolinol hydrochloride (m. 234°, with 1 mol. H₂O). The free bases (XII and XIII) could be obtained with K₂CO₃. Hydrogenation and recrystallization from EtOH or dilute HCl gave from XII 94% 1-(4-hydroxy-3-methoxyphenyl)-6-methoxy-1,2,3,4-tetrahydro-7-isoquinolinol hydrochloride (m. 182°), and from XIII 92% 1-(4-hydroxy-3,5-dimethoxyphenyl)-6-methoxy-1,2,3,4-tetrahydro-7-isoquinolinol hydrochloride (m. 150°, with 1 mol. H₂O). The free bases (XIV and XV) were obtained by K₂CO₃ treatment. Pd dehydrogenation gave from XI 90% 7-benzoyloxy-6-methoxy-1-phenylisoquinoline (XVI) (oil); from XIV 50% 1-(4-hydroxy-3-methoxyphenyl)-6-methoxy-7-isoquinolinol (hydrochloride, from EtOH-2N HCl, m. 240°; picrate, m. 220°); and from XV 56% 1-(4-hydroxy-3,5-dimethoxyphenyl)-6-methoxy-7-isoquinolinol (hydrochloride, from dilute HCl, m. 217°; picrate, m. 242-3°). Hydrolysis of XVI with aqueous EtOH-NaOH gave 75% 6-methoxy-1-phenyl-7-isoquinolinol (hydrochloride, m. 145-7°; picrate, m. 221-2°). 4-Benzylloxy-3,5-dimethoxybenzoic acid (XVII) (55.6%, m. 155-7° from EtOH-H₂O) was prepared from 2 g. syringic acid with PhCH₂Cl and KOH in EtOH. XVII formed 4-benzylloxy-3,5-dimethoxybenzoyl chloride (85%, m. 45°) with SOCl₂ at 50-70°. Syringaldehyde (XVIII) (48%, m. 110-12°, from H₂O) was prepared from 6.2 g. 5-methoxyprotocatechualdehyde with 12.6 g. Me₂SO₄ in 40 ml. H₂O containing 9.3 g. NaOH, then acidification with HCl. XVIII sodium salt gave 62.5% 4,3,5-PhCH₂O(MeO)C₆H₃CHO (XIX) (m. 63° from EtOH) with PhCH₂Cl in xylene. XIX (3.2 g.) in 25 ml. absolute

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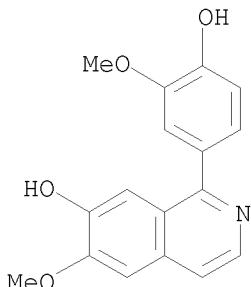
EtOH with 0.8 g. MeNO₂, 0.13 g. MeNH₂.HCl, and 0.1 g. Na₂CO₃ was heated 24 hrs. at 40° to give 65% 4,3,5-PhCH₂O (MeO)₂, C₆H₃CH:CHNO₂ (m. 133° from C₆H₆-EtOH). [3,4-MeO(PhCH₂O)C₆H₃]₂NH.HCl (XX) (m. 205-10° from EtOH) was prepared two ways: (A) 0.5 g. 3,4-MeO(PhCH₂O)C₆H₃CH:CHNO₂ was dissolved in 17 ml. HOAc plus 12 ml. C₆H₆. The solution was dropped into 50 mg. PtO₂ in 3 ml. HOAc under H. After taking up 150 ml. H, the solution was filtered and evaporated to 20 ml. under reduced pressure. Addition of concentrated HCl precipitated 51% XX; (B) 1 g. 3,4-MeO(PhCH₂O)C₆H₃CH₂CH:NOH was dissolved in 35 ml. EtOH and added to 50 mg. PtO₂ in 5 ml. EtOH under H. After absorption of 165 ml. H, XX (38%) was recovered as in A. XX (1 g.) was heated 3 hrs. at 130-40° with 14 ml. 38% formalin, the mixture was cooled and 2N HCl added to give 80% 4,4'-bisbenzyloxy-3,3'-dimethoxy-N-methyldiphenethylamine hydrochloride (m. 176-8°, from EtOH containing concentrated HCl; 1/2 mol. H₂O of crystallization).

XX (0.5 g.) on hydrolysis with 10 ml. concentrated HCl in 10 ml. EtOH gave 88% 4,4'-iminodiylenediguaiacol hydrochloride (m. 205-8°, from concentrated HCl). All the isoquinolines, phenethylamines, and intermediates showed 1/5 to 1/20 the spasmolytic activity of papaverine.

IT 855737-32-5, 7-Isoquinolinol,
1-(4-hydroxy-3-methoxyphenyl)-6-methoxy-
(and salts)

RN 855737-32-5 HCPLUS

CN 7-Isoquinolinol, 1-(4-hydroxy-3-methoxyphenyl)-6-methoxy- (CA INDEX NAME)



L13 ANSWER 262 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1955:84244 HCPLUS
DOCUMENT NUMBER: 49:84244
ORIGINAL REFERENCE NO.: 49:15886c-i,15887a-h
TITLE: Dimeric propenyl phenol ethers. XIX. The products obtained from diisohomogenol by oxidation with chromic acid
AUTHOR(S): Muller, Alexander; Lempert-Sreter, Magda;
Karczag-Wilhelms, Adrienne
CORPORATE SOURCE: Univ. Budapest
SOURCE: Journal of Organic Chemistry (1954), 19, 1533-47
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 49, 5459f. Because of the results obtained by Doering and Berson (C.A. 44, 5859c), the intermediates of the CrO₃ oxidation of diisohomogenol

have been reinvestigated. 1-(3,4-Dimethoxyphenyl)-2-methyl-3-ethyl-5,6-dimethoxy-2-indene (dipicrate, black needles, m. 109-11°) (10 g.) is refluxed 4 h. with 6 g. KOH in 100 cc. Me₂CHOH, 500 cc. H₂O is added, and the mixture extracted with Et₂O, giving 3 g. 1-indene isomer (I), long needles, m. 97-8°. I gives a reddish violet color with Br-AcOH. Hydrogenation of 2 g. I in AcOEt-EtOH (1:3) 50 min. with Pd-C gives 1.4 g. β-racemate of 1-(3,4-dimethoxyphenyl)-2-methyl-3-ethyl-5,6-dimethoxyindan, m. 105-6°. Adding (2 h.) 0.9 g. CrO₃ in 2 cc. H₂O and 8 cc. AcOH to 1.4 g. I in 40 cc. AcOH, keeping the mixture 2 days at 20°, and extracting with C₆H₆ gives 0.9 g. 3,3',4,4'-tetramethoxy-6-α-acetopropylbenzophenone (II), large cubes, m. 155-7°. Adding (3 h.) 675 g. red lead in small portions to 188 g. isohomogenol in 700 cc. AcOH at 50-5°, stirring the mixture 1 h., and extracting it with C₆H₆ give 153 g. yellow oil, b₃ 170-90°, which, refluxed with 500 cc. 25% H₂SO₄ 6 h. with stirring and extracted with C₆H₆, give 43% 3,4-dimethoxyphenylacetone (III), b₈ 165-70° (oxime, small silky needles, m. 62.5-3°; semicarbazone, slender needles, m. 176-7°). Adding 132 g. EtBr dropwise with cooling to 114 g. III in 580 cc. EtOH containing 16.1 g. Na dissolved, keeping the mixture 2 h. at 20°, refluxing it 3 h., distilling off 300 cc. EtOH, adding H₂O, and extracting with Et₂O give 39% α-(3,4-dimethoxyphenyl)propyl Me ketone, b_{0.05} 110-13° [semicarbazone, silky needles, m. 151-2°; oxime (IV), viscous oil, b_{0.06} 150-6°, needles, m. 78-80°]. Adding 5 g. Na to 4.6 g. IV in 40 cc. boiling EtOH, refluxing the mixture 15 min., pouring it onto ice, and extracting with Et₂O give 50% β-amino-γ-(3,4-dimethoxyphenyl)pentane (V), b_{0.1} 98-101° (HCl salt, rosettes, m. 143°). Adding (0.5 h.) 6 g. veratroyl chloride in 30 cc. Me₂CO to a refluxing solution of 6 g. V and 10 g. powdered K₂CO₃ in 25 cc. Me₂CO with stirring, diluting the mixture with H₂O, and extracting with EtOAc give 91% β-(3,4-dimethoxy-benzamido)-γ-(3,4-dimethoxyphenyl)pentane (VI), needles, m. 137-9°. Refluxing 3.85 g. VI in 80 cc. PhMe with 8 cc. POCl₃ 1.5 h., decomposing the mixture with ice, extracting the PhMe layer with concentrated HCl, adding the acid extract to the original aqueous solution, making it alkaline, and extracting it with ether give 60% 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxy-3,4-dihydroisoquinoline (VII), needles, m. 109° (HCl salt, greenish yellow needles, m. 219-20°). Heating an intimate mixture of 1.4 g. VII and 0.4 g. 5% Pd-C slowly to 200°, keeping it 45 min. at 200°, and extracting with ether give 0.9 g. 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisoquinoline (VIII), silky needles, m. 156-7°, purified via its picrate, bright yellow needles, m. 220-1°. Passing SO₂ into 5 g. VIII N-oxide [prepared from II and H₂NOH, small needles, m. 221-3°, (HCl salt, large yellow prisms, m. 203°)], in 200 cc. AcOH 4 h. at 100°, adding 200 g. ice, and making the mixture alkaline with NH₄OH give 3.2 g. VIII. Saturating 2 g. 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisochromenyl (IX) chloride (or sulfate) in 50 cc. absolute EtOH with NH₃ at 0°, keeping the mixture 12 h., distilling off 30 cc. EtOH, adding ice, and extracting with Et₂O also give VIII [oxalate, clusters of needles, m. 110° (decomposition); nitrate, yellow needles, m. 195-7° (decomposition); HCl salt, prisms, m. 208°, sulfate, light greenish yellow needles, m. 131-2° (air-dry) (decomposition), m. 237-8° (dried at 100°/14 mm.)]. Warming 5 g. IX sulfate in 100 cc. H₂O 1 h. gives 3.9 g. 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-

dimethoxyisochromenol (X), flat prisms, m. 156°, which, recrystd. from EtOAc, gives II, big cubes, m. 156°. Adding (0.5 h.) in small portions 2 g. finely powdered IX sulfate to 0.9-1 g. LiAlH₄ in 100 cc. Et₂O, decomposing the mixture with 5% HCl, and extracting with Et₂O give 0.9 g. 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisochromene, m. 105°, which, hydrogenated in AcOH with Pd-C, gives the diastereoisomer A of the corresponding isochroman, needles, m. 108-9°. Hydrogenating 7.7 g. II in 160 g. AcOH 4 h. gives 3 g. diastereoisomer B, flat needles, m. 97-8° (occasionally m. 104-6°). Both isomers decolorize Br-AcOH, give purple-violet color with concentrated H₂SO₄ from which colorless needles, m. 173°, sep.; fail to react with Ac₂O or H₂NNHCONH₂.HCl; and oxidized with CrO₃, give 53% and 55% II. Hydrogenation of the primary oxidation product (cf. C.A. 38, 2951.9) of diisoeugenol diacetate in AcOH gives 2.1 g. 1-(3-methoxy-4-acetoxyphenyl)-3-methyl-4-ethyl-6-methoxy-7-acetoxyisochroman, slender needles, m. 114°. Treating 1 g. 3,3',4,4'-tetramethoxy-6-propionyl benzophenone (XI) (cf. C.A. 39, 2745.1) in 3 cc. AcOH with 0.5 cc. concentrated H₂SO₄ in 1 cc. AcOH a few min. causes the crystallization of deep red needles; the mixture is filtered and diluted with 10 cc. H₂O, giving 0.1 g. 2,3,6,7-tetramethoxy-9-hydroxy-9-ethylanthrone, m. 143°, which, warmed with H₂O in 50% AcOH and 2 drops H₂O₂ gives 2,3,6,7-tetramethoxyanthraquinone, m. 339-42°. Warming 1 g. XI in 20 cc. EtOH with 0.8 cc. N₂H₄.H₂O gives 0.9 g. 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxyphthalazine, fine needles, m. 200-1° [picrate, canary-yellow needles, m. 199-201° (decomposition)]. Refluxing 0.3 g. 3,4'-dimethoxy-6-propionylbenzophenone, m. 117° (cf. C.A. 38, 4921.6) with 0.2 g. N₂H₄.H₂O in 2 cc. EtOH 5 min. gives 1-(p-methoxyphenyl)-4-ethyl-7-methoxyphthalazine.HCl, rosettes of slender needles, m. 93° (free base, needles, m. 136°; picrate, yellow needles, m. 179°). Adding dropwise 7 g. CrO₃ in 50 cc. H₂O to 25 g. IX sulfate in 140 cc. warm AcOH and 350 cc. H₂O, stirring the mixture 10 min., and cooling give 35% 2,3,6,7-tetramethoxy-9-acetyl-9-ethylanthrone (XII), sturdy prisms, m. 199-201°. Reduction of 1 g. XII in 10 cc. dioxane with 0.4 g. LiAlH₄ gives 0.09 g. 2,3,6,7-tetramethoxy-9-ethylanthracene, flat needles, m. 232°, which is also obtained when 1 g. 2,3,6,7-tetramethoxy-9-ethylanthrone (XIII) is refluxed with 0.4 g. LiAlH₄ in 50 cc. Et₂O, or when 2 g. XII is treated in 6 cc. AcOH with 1 cc. concentrated H₂SO₄ and the brick-red prisms, 2,3,6,7-tetramethoxy-9-ethyl-10-anthrolcarbenium sulfate (XIV), formed is reduced with LiAlH₄ at 30°, or when 2.8 g. 3,3',4,4'-tetramethoxydiphenylmethane in 40 cc. CS₂ is stirred with 0.7 g. EtCHO and 1.4 g. BF₃, the mixture kept 1 h. at 20°, and 2 h. at 100° (dipicrate, black cubes, m. 170-1°). Treating freshly prepared XIV from 5 g. XII with 100 cc. 96% MeOH at 20° gives 3.5 g. XIII, needles, m. 183-4°; when XIV is decomposed with H₂O pale yellow needles, m. 182-3°, resolidifying at 190° and remelting 225-35°, are obtained. Refluxing 2.7 g. XIII in 27 cc. dioxane with EtMgBr (from 3.27 g. EtBr) 40 h. and decomposing the mixture with HCl give 2.2 g. 2,3,6,7-tetramethoxy-9,10-diethylanthracene, slender needles, m. 236-47° (picrate, black needles, m. 182°). A corrected scheme for the degradation of IX sulfate is proposed.

IT 15462-86-9P

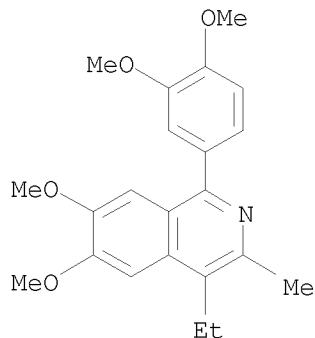
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Dimeric propenyl phenol ethers. XIX. The products obtained from

STN

diisohomogenol by oxidation with chromic acid)
RN 15462-86-9 HCAPLUS
CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl-,
compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

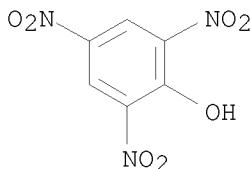
CM 1

CRN 1616-49-5
CMF C22 H25 N 04



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 263 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1955:53526 HCAPLUS
DOCUMENT NUMBER: 49:53526
ORIGINAL REFERENCE NO.: 49:10280f-i,10281a-i,10282a-i,10283a-d
TITLE: Hypotensive methoxyisoquinolines
AUTHOR(S): Walker, Gordon N.
CORPORATE SOURCE: Natl. Heart Inst., Bethesda, MD
SOURCE: Journal of the American Chemical Society (1954), 76, 3999-4003
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Dehydronorcoralydine iodide (I) was synthesized. The HCl salts of

3-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline (II),
 1-methyl-4-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline (III),
 1-methyl-4-phenyl-6,7-dimethoxyisoquinoline (IV),
 1-methyl-6,7-dimethoxyisoquinoline (V), and
 5-methyl-2,3,10,11-tetramethoxybenzo[a]-phenanthridine (VI) were prepared by
 the POCl₃ cyclization of the appropriate amides, dehydrogenation, and
 treatment with HCl. These compds. elicited a lowering of the blood
 pressure in normal dogs. N-(3,4-Dimethoxyphenylacetyl)homoveratrylamine
 (40 g.) refluxed 3 h. with 100 cc. POCl₃ in 800 cc. PhMe, the mixture
 treated with excess alc. KOH, and diluted with H₂O, and the product
 triturated with MeOH gave 30 g. (76%)
 1-(3,4-dimethoxybenzoyl)-6,7-dimethoxy-3,4-dihydroisoquinoline
 (3,4-dihydropapaveralidine) (VII), m. 185-9° (recrystd. from EtOAc,
 colorless crystals, m. 190-2°) (all m.ps. are corrected), λ_{maximum}
 6.03, 6.25-6.40 μ . VII (30 g.) in 250 cc. glacial AcOH hydrogenated at
 80° and 40 lb. pressure over 4.5 g. 10% Pd-C 5 h. (the catalyst was
 renewed twice during this period), the mixture filtered, the AcOH evaporated,
 the residual viscous oil dissolved in Et₂O-MeOH, the solution saturated with
 cooling with HCl, and the resulting crystals triturated with absolute EtOH and
 dried in air yielded 22.2 g. (67%) 1,2,3,4-tetrahydropapaverine (VIII) HCl
 salt, colorless crystals, m. 195-206° [recrystd. from MeOH, m.
 212-14° (decomposition)]. VIII.HCl (21 g.) in 300 cc. H₂O and 7 cc.
 concentrated HCl treated with 20 cc. CH₂O, the mixture heated 1 h. on the steam
 bath, the solution diluted with 400 cc. H₂O, cooled, treated with excess KOH,
 refrigerated overnight, and filtered, the filter residue triturated with
 150 cc. warm MeOH, the MeOH extract evaporated, and the residue recrystd. from

75

cc. MeOH yielded 7.3 g. (37%) crude product, m. 151-6°, which
 recrystd. from MeOH gave pure norcoralydine (IX) hemihydrate, colorless
 crystals, m. 159-61°; the MeOH-insol. crystals (8.0 g., 41%), m.
 174-97° (decomposition), recrystd. from EtOAc gave 5.6 g. unidentified
 product, slightly greenish crystals (X), m. 202-5° [recrystd. m.
 203-6° (partial decomposition)], λ_{maximum} 2.82-2.85, 7.2, 9.1 μ .
 IX and X showed very similar IR spectra. IX (2.0 g.) treated in 300 cc.
 absolute EtOH with 5.5 g. iodine, the mixture refluxed 4 h., cooled, and
 filtered, the filter residue triturated several times with warm EtOAc, the
 resulting deep red complex, decomposing 223-6°, which could not be
 recrystd. because of decomposition, warmed with aqueous NaHSO₃, and the
 resulting

yellow crystals washed with dilute HCl and H₂O, dried in air, and recrystd.
 from MeOH gave 1.4 g. I, yellow crystals, m. 222.5-26° (decomposition)
 (varied with rate of heating), which appeared to be solvated. X treated
 with iodine in the same manner, and the resulting red complex, decomposing
 222.5-26°, treated with aqueous NaHSO₃ yielded I, m. 252-4°
 (decomposition) (from MeOH); mixed m.p. with I from IX, 252-5°
 (decomposition). I caused with 1.0 mg./kg. dog a slight and with 31 mg./kg. a
 marked fall of the blood pressure, with 15 mg./kg. a partial epinephrine
 block, with 7 mg. a partial TMA block; the fatal dose was 63 mg./kg.; it
 caused also tachycardia. Homoveratroyl chloride treated with veratrole in
 the presence of AlCl₃ in CS₂, and the mixture distilled gave 31%
 3,3',4,4'-tetramethoxydeoxybenzoin (XI), colorless crystals, m.
 104-6° (from MeOH), b1.0 240-70°;
 2,4-dinitrophenylhydrazone, red-orange crystals, m. 197-9° (from
 EtOAc). XI treated with NH₂OH.HCl in pyridine gave the oxime of XI,
 colorless crystals, m. 129-31°; the hydrogenation of the oxime in
 EtOH and EtOAc over Pd-C gave products which were not identical with

α,β -di(3,4-dimethoxyphenyl)ethylamine (XII). 3,4-(MeO)₂C₆H₃CHO (81 g.), 101 g. 3,4-(MeO)₂C₆H₃CH₂CO₂H, 50.5 g. KOAc, and 230 cc. Ac₂O refluxed 2 h., the solution diluted with 100 cc. MeOH and 2000 cc. H₂O, and the precipitate washed with H₂O, pressed dry, and triturated with Et₂O gave 98 g. (58%) 3,4-(MeO)₂C₆H₃CH:[3,4-(MeO)₂C₆H₃] CO₂H (XIII), colorless crystals, m. 204-13° (recrystd. from EtOAc, m. 216-17°). XIII in glacial AcOH hydrogenated at 70° over 5% Pd-C, the mixture filtered, the filtrate evaporated, and the crude product (100%) recrystd. from MeOH gave α,β -di(3,4-dimethoxyphenyl)propionic acid (XIV), colorless crystals, m. 143-5°. XIV (83 g.) esterified with absolute EtOH in the presence of 5% concentrated H₂SO₄ yielded 73 g. (81%) crude Et ester (XV) of XIV, oil. BzCl (81.5 g.), 69.5 g. veratrole, and 89 g. AlCl₃ in 300 cc. CS₂ condensed in the usual manner, the resulting complex decomposed with ice and H₂O, and the neutral product recrystd. from MeOH in 2 crops yielded 83 g. (68%) 3,4-(MeO)₂C₆H₃Bz (XVI), m. 98-100°; 2,4-dinitrophenylhydrazone, red crystals, m. 256-7° (from EtOAc). XVI (41.3 g.), 36 g. BrCH₂CO₂Et, 50 g. activated Zn (30 mesh), and 500 cc. dry C₆H₆ refluxed 4 h., the mixture decomposed with dilute AcOH, the neutral product isolated in the usual manner and hydrogenated in glacial AcOH at 80° 1 h. over 10% Pd-C at 40 lb. pressure, the mixture filtered, and the filtrate evaporated gave 100% crude 3,4-(MeO)₂C₆H₃CHPhCH₂CO₂Et, orange oil, suitable for further conversions. XI (23 g.), 200 cc. HCONH₂, 100 cc. 90% HCO₂H, and 50 g. HCO₂NH₄ distilled until the reflux temperature reached 165°, the mixture refluxed 9 h., cooled, and diluted with 3000 cc. H₂O, and the crystalline precipitate washed with H₂O and recrystd. from MeOH yielded 14 g. (56%) N-CHO derivative (XVIII) of XII, m. 138-41° (recrystd. from MeOH, m. 141-3°), λ_{maximum} 2.95, 5.94 μ . XIV refluxed 3 h. with 2 parts by weight anhydrous N₂H₄, the solution cooled and poured into 20 vols. ice water, and the crystalline precipitate washed with several portions H₂O and dried in vacuo at room temperature yielded the hydrazide of XIV, colorless crystals, m. 140-2° (from MeOH). [3,4-(MeO)₂C₅H₃CHCH₂CONHNH₂, colorless crystals, m. 240-2°, was obtained similarly from [3,4-(MeO)₂C₆H₃]₂CHCH₂CO₂Et; in the same manner was prepared 3,4-(MeO)₂C₆H₃CHPhCH₂CONHNH₂, colorless crystals, m. 113-15° (from MeOH), from XVII; and 1-(3,4-dimethoxyphenyl)-2-carboxy-6,7-dimethoxytetralin hydrazide (XIX), colorless, hygroscopic crystals, m. 180-1° (from MeOH, dried in vacuo at 100°), from the Et ester of the corresponding acid. Each of the hydrazides showed IR absorption bands at 2.94 and 5.98 μ . The acid hydrazide (0.1 mol) in 300 cc. glacial AcOH, 200 cc. concentrated HCl, and 200 cc. H₂O treated with 600 cc. Et₂O to form a 2nd phase, the mixture treated with cooling and stirring with 20 g. NaNO₂ gradually during 0.5 h., diluted with 1 l. ice water, and shaken, the organic layer washed 4 times with H₂O, with 3% aqueous NaOH until alkaline, and then with dilute AcOH, aqueous NaHCO₃, and H₂O, dried with MgSO₄, treated immediately with 75 cc. glacial AcOH and 50 cc. Ac₂O, and cautiously distilled to remove the Et₂O, the residual liquid refluxed 2 h., the excess reagent evaporated, the residue treated with an equal volume Et₂O containing a little Et₂O, and the product recrystd. gave the rearrangement product. In this manner were prepared the N-Ac derivative (XX) of XII, m. 148-65° (recrystd. from EtOAc, colorless crystals, m. 160-3°), in 61% from XIII, λ_{maximum} 2.94, 6.00 μ [XX gave hydrolyzed 4 h. with KOH in

aqueous ($\text{HOCH}_2\text{CH}_2\text{O}$)₂O XII, colorless crystals, m. 106-10° (from EtOAc)]; [3, 4-(MeO)2C6H3]2CHCH2NHAc (XXI), colorless crystals, m. 129-31°

(from MeOH), in 52% yield from XI, λ_{maximum} 2.94, 6.01 μ ;

3, 4-(MeO)2C6H3CHPhCH2NAC (XXII), colorless crystals, m. 154-6°

(from MeOH), in 46% yield from XVI; and

1-(3, 4-dimethoxyphenyl)-2-acetylaminio-6, 7-dimethoxytetralin (XXIII), m.

217-20° (recrystd. from MeOH, pale green crystals, m.

222-3.5°), in 73% yield from XIX, λ_{maximum} 2.90, 6.00 μ .

The appropriate amide and dry PhMe (volume equal to 40 times the weight of the amide in g.) boiled until solution occurred, the warm solution treated with POC13 (volume in cc. equal to twice the weight of the amide: the solution refluxed

2-3 h. after the spontaneous reaction subsided, cooled, diluted with 15 vols. pentane, and filtered, the precipitate dissolved in the min. amount hot absolute

EtOH, the hot solution treated with solid KOH until a strong alkaline reaction persisted, cooled, and diluted with cold H2O until no further separation occurred, the product extracted with Et2O-EtOAc (2-4 portions), and the extract washed with 2 portions H2O, dried, and evaporated at 70° gave the desired 3, 4-dihydroisoquinoline (XXIV). The XXIV, an equal weight 10% Pd-C, and p-cymene (volume in cc. equal to 100 times the weight of the XXIV) distilled

until the reflux temperature reached 175°, the residual mixture refluxed 2-4 h. and filtered hot, the filtrate recharged with the catalyst, refluxed 3 h., filtered, and evaporated, and the resulting isoquinoline recrystd.; if the product did not crystallize, it was dissolved in MeOHEtOAc and treated with dry HCl to give the crystalline HCl salt. XVIII (7.0 g.) cyclized in this manner, and the resulting brown, viscous oily

XXIV (3.0 g.) dehydrogenated and triturated with MeOH gave 1.2 g. (18%) 3-(3, 4-dimethoxyphenyl)-6, 7-dimethoxyisoquinoline (II), m. 204-9°

(recrystd. from MeOH, brilliant, pale-yellow leaflets, m. 212-14°), λ_{maximum} 6.15 μ ; HCl salt, yellow crystals, m. 232-5° (from

MeOH), λ_{maximum} 6.15 μ , showed at 50 mg./kg. a slow fall of the

blood pressure, at 15 mg./kg., partial TMA block; the fatal dose was above

50 mg./kg. II refluxed 3 h. with EtI did not give an ethiodide. XXI (4.5 g.) cyclized and the product triturated with MeOH yielded 3.5 g. (82%)

3, 4-dihydro derivative (XXV) of III, discolored crystals, m. 75-80°

(recrystd. from MeOH, colorless crystals, m. 87-9°),

$\lambda_{\text{CHCl}_3\text{max}}$. 6.14 λ , soluble in dilute HCl. XXV (3.5 g.)

dehydrogenated in the usual manner, and the product triturated with MeOH

yielded 1.4 g. (40%) III, crystals, m. 205-7° (recrystd. from MeOH,

pale greenish yellow crystals, m. 206-8°), $\lambda_{\text{CHCl}_3\text{max}}$. 6.14

μ ; HCl salt hemihydrate, pale yellow needles, m. 206-7°

(decomposition) (dried in vacuo at 80°), 3.0 mg./kg. and up caused a

sustained fall of the blood pressure, 31 mg./kg. gave epinephrine block

and TMA block and caused convulsions and tachycardia; the fatal dose was

above 63 mg./kg. III refluxed 1.5 h. with a large excess EtI, and the

gradually separating yellow crystals recrystd. from MeOH gave III.MeI, bright

yellow crystals, m. 219-23° (decomposition), which could not be analyzed

successfully because of its hygroscopic properties; 7.0 mg./kg. cause a

slight and 15 mg./kg. a marked fall of blood pressure; 7 mg./kg. gave an

epinephrine shock with rapid recovery and a partial TMA block, and also

caused tachycardia; the fatal dose was 76 mg./kg. XXII (19.5 g.) cyclized

gave 18 g. viscous, red oil (λ_{maximum} 5.80, 6.15 μ ; soluble in dilute

HCl); a 17-g. portion dehydrogenated in the usual manner, the resulting

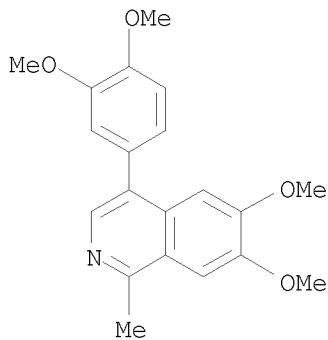
greenish glassy substance remaining after the evaporation of the p-cymene

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dissolved in MeOH-EtOAc, the solution treated with cooling with dry HCl, and the crystalline precipitate recrystd. from EtOAc containing the min. amount MeOH yielded 6.5 g. (33%) IV.HCl.0.5H₂O, m. 173-5° (recrystd. from EtOAc-MeOH, colorless needles, m. 183-5° (decomposition) (dried in vacuo at 80°); 7.0 mg. caused a moderate, transient fall of blood pressure, 31 mg./kg. gave a TMA and a partial epinephrine block, fatal dose above 57 mg. 3,4-(MeO)2C₆H₃(CH₂)₂NHAc (14.2 g.) cyclized gave 3.6 g. (26%) 1-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline (XXVI), m. 85-96° (recrystd. from cyclohexane, m. 102-4°), λ_{maximum} 6.15 μ , moderately soluble in H₂O. XXVI (3.2 g.) dehydrogenated gave a green glassy material which treated with HCl in MeOH-EtOAc and cooled yielded 2.5 g. (67%) V.HCl, m. 219-221° (decomposition) [recrystd. from MeOH-EtOAc, colorless crystals having a green cast, m. 226-8° (decomposition)]; 3.0 mg./kg. showed a slight and 31 mg. a moderate, sustained fall of blood pressure, 53 mg./kg. gave an epinephrine and a TMA block; the fatal dose was above 53 mg./kg. XXVI (7.2 g.) cyclized gave 6.2 g. (91%) discolored crystals, m. 157-60°, which recrystd. from EtOAc gave the 7,8,15,16-tetrahydro derivative (XXVII) of VI, colorless crystals with a green-yellow cast, m. 160-2°, $\lambda_{\text{CHCl3max}}$. 6.21, 6.07, 6.18 μ . Crude XXVII (2.3 g.) dehydrogenated and the product triturated with MeOH yielded 1.6 g. (70%) VI, crystals, m. 191-3°, $\lambda_{\text{CHCl3max}}$. 6.18 μ ; HCl salt, yellow needles, m. 224-5° (from MeOH), readily soluble in H₂O; 1.0 mg./kg. and up gave a moderate fall of blood pressure, 7.0 mg./kg. and up caused a partial epinephrine block, 15 mg./kg. a partial TMA block; the fatal dose was above 31 mg./kg. VI refluxed 3 h. with EtI gave the VI.MeI which warmed with MeOH gave VI. XXVII in glacial AcOH hydrogenated 1 h. at 40 lb. pressure and 70° over 5% Pd-C, and the resulting semicryst., hygroscopic material triturated with EtOAc, treated in MeOH-EtOAc with dry HCl, and recrystd. from MeOH gave 5,6,7,8,15,16-hexahydro derivative of VI, colorless crystals, m. 263-5°. XX (22 g.) refluxed 4 h. in 500 cc. dry PhMe with 40 cc. POCl₃, the product isolated in the usual manner, and the resulting partially crystallized material (11 g.) triturated and recrystd. with MeOH gave 4.5 g. colorless crystals, m. 157-9°; the filtrate evaporated gave a glassy residue; both products were free of N but seemed to contain a small amount nonnitrogenous impurity; λ_{maximum} 6.22-6.27 μ (doublet); the product was presumably (3,4-C₆H₃CH₂):2.

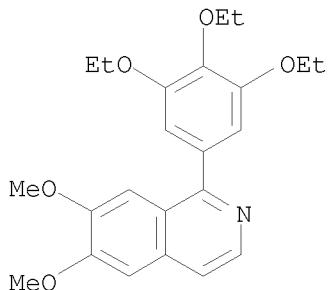
IT 102012-79-3, Isoquinoline,
4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-
RL: PREP (Preparation)
(and derivs.)
RN 102012-79-3 HCPLUS
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)

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OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

L13 ANSWER 264 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1954:53923 HCAPLUS
DOCUMENT NUMBER: 48:53923
ORIGINAL REFERENCE NO.: 48:9545h-i,9546a
TITLE: Action of octaverine, perparine, and papaverine on circulatory and respiratory systems
AUTHOR(S): Goldberg, A. A.; Shapero, M.
SOURCE: Journal of Pharmacy and Pharmacology (1954), 6, 236-45
CODEN: JPPMAB; ISSN: 0022-3573
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB In tests on rabbits octaverine (I) and perparine (II) have approx. twice the hypotensive activity of papaverine (III). The depressor activity of I is of longer duration than with II or III and there is no secondary rise in blood pressure above the normal level. III causes a slight decrease while I and II effect a substantial increase in the ventilation rate (respiratory rate + amplitude). I and II are 2 to 3 times as active as III in counteracting adrenaline-induced hypertension. I has a higher adrenolytic activity than II or III in mice. II is slightly less active while I is slightly more active than III in increasing the coronary flow in the perfused isolated heart.
IT 549-68-8, Octaverine
(effect on circulation and respiratory tract)
RN 549-68-8 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 265 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1954:49472 HCAPLUS
 DOCUMENT NUMBER: 48:49472
 ORIGINAL REFERENCE NO.: 48:8788f-i,8789a-e
 TITLE: Syntheses of isoquinoline derivatives. XXV. Migration
of the double bond of isoquinoline derivatives. 2
 AUTHOR(S): Kametani, Tetsuji; Ninomiya, Kichijiro
 CORPORATE SOURCE: Univ. Osaka
 SOURCE: Yakugaku Zasshi (1953), 73, 681-5
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB RAC ($R = 3,4-(MeO)C_6H_3$) (20 g.) in 60 ml. alc., 5.6 g. NaOH, and 52 ml. water treated with 16.8 g. $R'CHO$ ($R' = 3,4-CH_2C_6H_3$) in 60 ml. alc., the mixture stirred 1 hr., kept overnight at 0° , and the product filtered, washed with water, and recrystd. from alc. gives 28 g. (80.7%) $RCOCH:CHR'$ (IX), m. 144°; 10 g. IX on catalytic reduction in AcOEt with Ni (10 g. Raney Ni, 12 g. NaOH, and 48 ml. water) and H absorbs 737 ml. H to give 9.9 g. (98.4%) $RCOCH_2CH_2R'$ (X), m. 102°. A mixture of 3 g. Na in 50 ml. EtOH, and 10 g. X treated with 15 g. AmNO₂ in 100 ml. alc. and 200 ml. C₆H₆ at 0° , kept overnight, the solvent removed, the residue in water extracted with Et₂O, the aqueous layer neutralized with

10% HC_l, and the precipitate extracted with Et₂O gives 10.1 g. product (92.6%) which

yields veratric acid, m. 179°, and the mother liquor gives $RCOC(:NOH)CH_2R'$ (XI), m. 131°. XI (5 g.) in 210 ml. alc. and 3.5 ml. concentrated HC_l reduced with 5 g. Raney Ni and H gives 3 g. (62.5%) $RCH(OH)CH(NH_2)CH_2R'$, 1.8 g. of which in 10% NaOH treated with 0.91 g. BzCl, kept overnight, and extracted with AcOEt gives 1.6 g. (67.2%) $RCH(OH)CH(NHBz)CH_2R'$ (XII), m. 172°. XII (1 g.) in 10 ml. C₆H₆ and 5 g. POC₁₃ heated 2 hrs. on a water bath, and the product treated with petr. ether, extracted with alc. HC_l, and neutralized with 10% NH₄OH gives 0.5 g. (54.5%) $C_25H_{21}O_4N$ (XIIA), m. 68-83°; XIIA.0.5H₂PtCl₆, m. 150° (decomposition). Na in absolute alc., and 42 g. AcCH₂CO₂Et at 5° mixed with 70 ml. of a solution of 59 g. 3,4-CH₂C₆H₃COCl in 300 ml. C₆H₆ in the course of 3 hrs. gives 52 g. 3,4-CH₂C₆H₃COCHAcCO₂Et (XIII); a filtered solution of XIII in 500 ml. water heated 30 min. at 35-45° with 12 g. NH₄Cl and 35 ml. 10% NH₄OH and extracted with Et₂O gives 15 g. 3,4-CH₂C₆H₃COCH₂CO₂Et (XIV), m. 38-40°. XIV (30 g.) in 150 ml. 10% KOH and 150 ml. 99% alc. boiled 30 min., cooled, 100 ml. saturated NaCl solution added, the alc. removed, and 50 ml. water added gives

19 g. (91%) 3,4-CH₂C₆H₃Ac (XV), leaves, m. 83-6° (from dilute alc.). A mixture of 12 g. XV, 12 g. 3,4-(MeO)C₆H₃CHO, 210 ml. 99% alc., 3.6 g. NaOH, and 32 ml. water stirred 8 hrs. at 25°, kept overnight, and the precipitate filtered and washed with alc. gives 18 g. (78.9%) $R_2COCH:CHR$ (XVA), columns, m. 132-3.5° (from alc.). Catalytic reduction of 7 g. XVA in 230 ml. AcOEt with 5 g. Raney Ni gives 7.4 g. (93%) $R'COCH_2CH_2R$ (XVI), needles, m. 95-7° (from alc.). Na (3 g.) in 50 ml. absolute alc. treated with 10 g. XVI, 130 ml. C₆H₆, 80 ml. alc., and 15 g. AmNO₂, the mixture refluxed 2 hrs., kept overnight, and the product treated as usual give 10.9 g. $R'CH(OH)C(:NOH)CH_2R$ (XVII). Catalytic reduction of 5

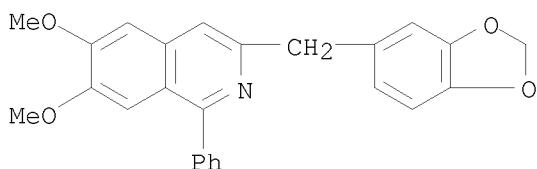
g. XVII in 210 ml. alc. with Pt-Pd mixture give 1.5 g. (31.2%) R'CH(OH)CH(NH₂)CH₂R (XVIIIA); 2.4 g. XVIIIA in 60 ml. C₆H₆ and 160 ml. 10% NaOH treated with 1.2 g. BzCl in 10 ml. C₆H₆ and the product treated as usual with AcOEt gives 2.8 g. (88.8%) R'CH(OH)CH(NHBz)CH₂R (XVIII), m. 153-9° (from petr. ether). XVIII (1 g.) in 10 ml. C₆H₆ and 5 g. POC₁₃ heated 3 hrs. on a water bath, the mixture treated with petr. ether as usual, and the residue extracted with 80 ml. 10% HCl and basified with 10% NH₄OH gives 0.1 g. C₂₅H₂₁O₄N (XVIIIB), needles, m. 180-3° (from alc.); the residue (insol. in 10% HCl) extracted with a mixture of 30 ml. alc. and 50 ml. 10% HCl, the extract basified with NH₄OH, the precipitate extracted with

Et₂O, the Et₂O removed, and the residue recrystd. from alc. gives XVIIIC; the mother liquor taken up in alc.-HCl and precipitated with NH₄OH gives C₂₅H₂₁O₄N (XVIIIC), m. 75-85° [XVIIIC.0.5HAuCl₄.2H₂O, m. 98-130° (decomposition)]. The structures of the cyclized products, XIIA, XVIIIB, and XVIIIC, are discussed.

IT 855650-08-7P, Isoquinoline, 6,7-dimethoxy-1-phenyl-3-piperonyl-
RL: PREP (Preparation)

RN 855650-08-7 HCPLUS

CN Isoquinoline, 3-(1,3-benzodioxol-5-ylmethyl)-6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 266 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1954:49471 HCPLUS

DOCUMENT NUMBER: 48:49471

ORIGINAL REFERENCE NO.: 48:8788a-f

TITLE: Syntheses of isoquinoline derivatives. XXIV. Migration of the double bond of isoquinoline derivatives. 1

AUTHOR(S): Kametani, Tetsuji; Iida, Hideo

CORPORATE SOURCE: Univ. Osaka

SOURCE: Yakugaku Zasshi (1953), 73, 677-80

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 48:49471

AB cf. C.A. 47, 10539c. 3,4-(MeO)₂C₆H₃COCH:CHPh (I) (30 g.) in 250 ml. AcOEt reduced with Pd-C and H gives 22 g. (75%) 3,4-(MeO)₂C₆H₃COCH₂CH₂Ph (I), plates, m. 73°. I (10 g.) in 10 ml. C₆H₆, 2 g. Na in 30 ml. alc., and 12 g. AmONO kept overnight, the precipitate filtered, dissolved in a small amount of water, neutralized with HCl, the precipitate (1 g.) filtered,

the

filtrate concentrated, Et₂O added, the mixture extracted with water, and the aqueous layer

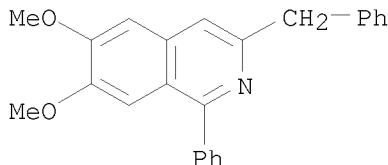
neutralized with 10% HCl and extracted with Et₂O gives 7.5 g.

3,4-(MeO)₂C₆H₃COC(:NOH)CH₂Ph (II), sirup. II (5 g.) in 200 ml. alc. and 5

ml. concentrated HCl reduced with 0.3 g. Pt-Pd mixture and H 8 hrs. absorbs 680 ml. H and the product treated as usual gives 2.1 g.
 3,4-(MeO)2C6H3CH(OH)CH(NH2)CH2Ph in sirupy form; this with 1.3 g. BzCl gives 2.6 g. (91%) 3,4-(MeO)2C6H3CH(OH)CH(NHBz)CH2Ph (III). III (2.6 g.) in 20 ml. C6H6 and 15 g. POC13 heated 1.5 hrs. on a water bath, petr. ether added, and the mixture kept overnight, extracted with alc. HCl, made alkaline, and extracted with AcOEt gives 2.2 g. 1-phenyl-3-benzyl-6,7-dimethoxyisoquinoline (IV); IV.0.5H2PtCl6.5.5H2O, m. 179-80° (from dilute AcOH). Na (2 g.) in 30 g. alc., 10 g. IA in C6H6, and 12 g. AmNO2 kept 2 days, the precipitate filtered, washed with Et2O, taken up in a small amount of water, neutralized with dilute HCl, and the precipitate filtered, washed with water, and recrystd. from petr. ether-C6H6 (3:1) gives 2 g.
 3,4-(MeO)2C6H3CH2C(:NOH)Bz (V), silky needles, m. 87-9°. Catalytic reduction of 2.1 g. V in alc. with Pd-C and H gives 0.9 g.
 3,4-(MeO)2C6H3CH2CH(NH2)CH(OH)Ph (VI), sirupy; 0.9 g. VI in Et2O and 10% NaOH treated with 0.5 g. BzCl in Et2O, and the product extracted with C6H6 and washed with dilute HCl, NaHCO3, and water gives 0.7 g.
 3,4-(MeO)2C6H3CH2CH(NHBz)CH(OH)Ph (VII) (hemihydrate, m. 179-80°). VII (0.5 g.) in 17 ml. C6H6 and 3 ml. POC13 heated 2 hrs. on a water bath, the product treated as usual, taken up in alc. HCl, neutralized with 10% NH4OH, and the precipitate filtered and washed with water gives 0.4 g. 1-phenyl-3-benzylidene-6,7-dimethoxy-3,4-dihydroisoquinoline (VIII), m. 84-7° (from dilute alc.); VIII.0.5H2PtCl6.H2O, m. 220-1° (decomposition). On catalytic reduction in 40 ml. alc. with 0.1 g. PtO2 0.6 g. VIII absorbs 190 ml. H, and the product extracted with alc.-HCl, neutralized with 10% NaOH, and the precipitate filtered and washed with water gives the 3-benzyl analog of VIII, m. 102° (decomposition); C24H23O2N.0.5H2PtCl6.0.5H2O, m. 145-8°.

IT 412337-92-9P, Isoquinoline, 3-benzyl-6,7-dimethoxy-1-phenyl-
 RL: PREP (Preparation)
 (preparation of)

RN 412337-92-9 HCPLUS
 CN Isoquinoline, 6,7-dimethoxy-1-phenyl-3-(phenylmethyl)- (CA INDEX NAME)



L13 ANSWER 267 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1954:47315 HCPLUS
 DOCUMENT NUMBER: 48:47315
 ORIGINAL REFERENCE NO.: 48:8413g-i
 TITLE: Comparative spasmolytic activities of octaverine,
 perparine, and papaverine
 AUTHOR(S): Goldberg, A. A.; Shapero, M.
 SOURCE: Journal of Pharmacy and Pharmacology (1954),
 6, 171-7

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CODEN: JPPMAB; ISSN: 0022-3573

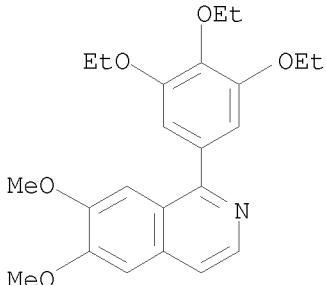
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Octaverine (I) and perparine (II), 2 synthetic analogs of papaverine (III), have about one-half the acute toxicity of III as shown by the combined LD₅₀ figures, the min. convulsive doses and the min. doses required to diminish reflexes and establish lateral decubitus in mice. I is 4 times, and II is twice as active as III in suppressing the spontaneous contractions of rat uterus. All 3 alkaloids have the same activity against BaCl₂-induced spasm in isolated guinea-pig ileum. I and III possess the same activity against spasm provoked by histamine or pilocarpine; II has half the activity of III against histamine spasm and twice the activity of III against pilocarpine spasm. Orally administered III has no action against histamine bronchospasm in guinea pigs; both I and II show definite but little activity under comparable conditions.

IT 549-68-8, Octaverine
(antispasmodic activity of)

RN 549-68-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 268 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1954:11113 HCPLUS

DOCUMENT NUMBER: 48:11113

ORIGINAL REFERENCE NO.: 48:2067c-i,2068a

TITLE: Synthesis of bisquinolines derivatives on the model of natural alkaloids. I. Isoquinoline derivatives of diphenyl ether

AUTHOR(S): Marini-Bettolo, G. B.; Chiavarelli, S.

CORPORATE SOURCE: Ist. super. sanità, Rome

SOURCE: Rendiconti Istituto Superiore di Sanità (Italian Edition) (1952), 15, 1041-53

CODEN: RISSAF; ISSN: 0370-5811

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB p-PhOC₆H₄COMe (159 g.), prepared according to Kipper [Ber. 38, 2490(1905)], 67.5 ml. morpholine, and 24 g. S refluxed 15 hrs., diluted with H₂O, extracted with Et₂O, and the solvent distilled off; yielded 215 g. crude morpholide, m. 87° (from EtOH), p-PhOC₆H₄CH₂CSOH, m. 87° (EtOH). The morpholide (215 g.) of p-PhOC₆H₄CH₂CO₂H (I) refluxed with 1 l. 20% KOH, diluted with 2 vols. H₂O, acidified with concentrated HCl, and the product taken up in Et₂O yielded 117 g. crude I, m. 78° (from petr. ether).

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PhCH₂CH₂NH₂ (12 g.), and 23 g. crude I refluxed 5 hrs. at 180-90 and the product distilled yielded 20 g. p-PhOC₆H₄CH₂CONHCH₂CH₂Ph, m. 84-5° (from petr. ether). The amide (20 g.), 20 g. P2O₅, and 100 ml. xylene refluxed 20 hrs., the solvent discarded, the residue taken up in H₂O, and the solution made strongly alkaline with 20% NaOH, and extracted with Et₂O yielded

6.4 g. 1-(p-phenoxybenzyl)-3,4-dihydroisoquinoline (II), b0.6 204-14°. II (1 g.) refluxed 4 hrs. in 25 ml. tetrahydronaphthalene with 0.3 g. 5% Pd-C, the mixture filtered, acidified with HCl, and the precipitate

filtered off yielded 0.6 g. 1-(p-phenoxybenzyl)isoquinoline-HCl, m. 207° (from EtOH). II (1.5 g.) in 25 ml. EtOH, with 0.5 g. Pd black took up the theoretical amount of H in 2.5 hrs.; after filtration from the catalyst, 1.1 g. 1(p-phenoxybenzyl)-1,2,3,4-tetrahydroisoquinoline was recovered from the EtOH [picrolonate, m. 230° (from EtOH)]. (p-AccC₆H₄)₂O (Kipper, loc. cit.) (380 g.) refluxed 19 hrs. at 170-80° with 221 g. morpholine and 78.5 g. S, and the product taken up in MeOH, yielded 371 g. morpholide, m. 154°, of (p-HOCC₆H₄)₂O (III). To this in 1050 ml. concentrated HOAc was added 157 ml. concentrated H₂SO₄ in

226 ml. H₂O, the mixture refluxed, cooled diluted with 4 l. H₂O, and the precipitate

filtered, yielding 195 g., (p-HO₂CCH₂C₆H₄)₂O (IV), m. 207°. IV (12 g.), 20 g. homoveratrylamine and 150 ml. freshly distilled tetrahydronaphthalene were refluxed under N atmospheric, at 200-30° 100 ml. of H₂O-tetrahydronaphthalene azeotrope distilled off, and the residue diluted with 1 l. PhMe, yielding 27 g. bis(homoveratrylamide of IV, m. (pure) 99°. The amide (19 g., recrystd. from PhMe) refluxed in 100 ml. CHCl₃, 40-5 ml. solvent distilled off, 19 g. PC15 added, the mixture was heated 6 hrs. at 30°, then 6 hrs. at 40°, decomposed with H₂O, the CHCl₃ distilled off, 10% NaOH added to the residue, and the solution extracted

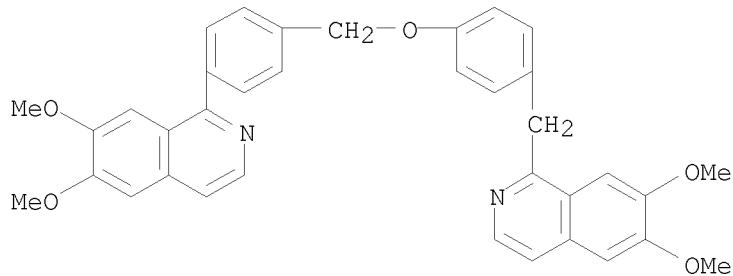
with CHCl₃, yielded 7 g. p-benzoyloxybenzylbis[1,1'-(6,7-dimethoxy)-3,4-dihydroisoquinoline](1,1'-[oxybis(p-phenylenemethylene)]bis[3,4-dihydro-6,7-dimethoxyisoquinoline]) (V), m. 150-5°, reduces AgNO₃ at once and oxidizes in air. Attempted recrystn. of V gave p-benzoyloxybenzoylbis[1,1'-(6,7-dimethoxy)-3,4-dihydroisoquinoline](1,1'-[oxybis(p-phenylenecarbonyl)]bis[3,4-dihydro-6,7-dimethoxyisoquinoline]) (VI), m. 167-8°. VI (2 g.), 50 ml. tetrahydronaphthalene and 2 g. 5% Pd-C refluxed 6 hrs. under N, the catalyst removed, and the solvent distilled in vacuo; yielded an oily residue of p-benzoyloxybenzylbis[1,1'-(6,7-dimethoxy)isoquinoline] [picrate, m. 230°; HCl salt m. (decomposition) 166-7° (from anhydrous Et₂O)]. VI (2 g.), in 100 ml. 1:1 HCl reduced by H₂ with Pd black 4 hrs. gave p-benzoyloxybenzylbis[1,1'-(6,7-dimethoxy)-1,2,3,4-tetrahydroisoquinoline], m. (decomposition) 145-8° (HCl salt, m. 205-7°; picrate, m. 177-8°). The morpholide (1 g.) of III, suspended in 200 ml. dioxane, and refluxed 18 hrs. with 0.5 g. LiAlH₄ gave p-phenoxyphenyl-4,4'-bis[β-ethylene-N-morpholine], m. 207-8°; picrate, m. 177°.

IT 1082669-91-7P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Synthesis of bisquinolines derivatives on the model of natural alkaloids. I. Isoquinoline derivatives of diphenyl ether)

RN 1082669-91-7 HCPLUS

CN INDEX NAME NOT YET ASSIGNED



L13 ANSWER 269 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1953:58664 HCPLUS

DOCUMENT NUMBER: 47:58664

ORIGINAL REFERENCE NO.: 47:9975b-g

TITLE: N-Acyl-phenethylamines, and a new isoquinoline synthesis

AUTHOR(S): Ritter, John J.; Murphy, Francis X.

CORPORATE SOURCE: New York Univ., New York, NY

SOURCE: Journal of the American Chemical Society (1952), 74, 763-5

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 43, 2165i. $\text{CH}_2:\text{CHCH}_2\text{Ph}$ (I) (5.9 g.) and 5.2 g. PhCN at 10° treated gradually with 2.7 cc. H₂SO₄, the cooling bath removed, the mixture held below 60° by occasional cooling, and let stand overnight at room temperature, warmed briefly on the steam bath, poured into water, neutralized with Na₂CO₃, and filtered yielded 6.5 g.

N-benzoyl- α -methylphenethylamine, m. 131-3°. For other N-acyl analogs, PhCH₂CHMeNHCOR, R, % yield, and m.p. are: PhCH₂, 53, 113-15°; 3,4-(MeO)₂C₆H₃, 53, 114-20°; 3,4-(EtO)₂C₆H₃, 97, 149-51°. Amides or dihydroisoquinolines could not be obtained from safrole. Eugenol Me ether (II) (10.1 cc.) added to 6.2 cc. PhCN and 3.3 cc. H₂SO₄ at 20° with the mixture held at 60° during the addition (3-4 min.) and then let stand 2 days at room temperature yielded 2.8 g.

1-phenyl-3-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline-HCl, m. 259-63°. II (10.2 cc.) added to 9.8 g. veratronitrile in 15 cc. H₂SO₄ during 2 min. with the temperature held at 80°, and the mixture let stand 3 days at room temperature, yielded 11.5 g.

1-(3,4-dimethoxyphenyl)-3-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline (III), m. 138-9°; HCl salt m. 185-6° (decomposition).

1-p-MeOC₆H₄ analog of III, m. 104-5°. 3,4-(EtO)₂C₆H₃CN and II yielded 0.24 g. 1-[3,4-(EtO)₂C₆H₃] analog of III, m. 104°, and 3,4-(EtO)₂C₆H₃CONH₂. III (0.2 g.) and 0.2 g. 5% Pd-C in 10 cc. tetrahydronaphthalene refluxed 1 h. and the filtrates treated with 5 cc. dilute HCl yielded 0.15 g. 1-(3,4-dimethoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline-HCl.2H₂O, m. 197-8° (decomposition). PhCH₂CMe₂OH

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(4.5 g.) and 3.1 g. in 5 cc. AcOH treated with 2 cc. H₂SO₄, and the mixture let stand 4 h., poured onto ice, and neutralized with Na₂CO₃ yielded 6.4 g. N-benzoyl- α,α -dimethylphenethylamine, m. 112-13°.

For other compds. of the type PhCH₂CMe₂NHCOR, R, % yield, and m.p. are:

C₁CH₂, 87, 62.5-4°; Me, 84, 91.5-2°; vinyl, 90,

115-15.5°; H₂NOCCH₂, 78, 148.5-9.5°; Et, 100,

97.5-8.5°; Pr, 94, 59.5-60°; 3-pyridyl, 71, 91-3°;

p-O₂NC₆H₄CH₂, 93, 149-50°; o-tolyl, 74, 70-1°; PhCH₂, 86,

107-8°; p-MeOC₆H₄, 81, 119-21°;

2-hydroxy-4,6-dimethyl-3-pyridyl, 34, 175-7°; PhCH₂CH₂, 95,

65-6.5°; 3,4-(MeO)₂C₆H₃, 71, 99-101°; Ph₂CH, 50,

152-4°. tert-BuOH (2.2 g.) and 5.8 g. Ph₂CHCN in 6.5 cc. AcOH

stirred with 2 cc. concentrated H₂SO₄, and the mixture let stand overnight, poured

over ice, and neutralized with Na₂CO₃ yielded 8 g.

N-tert-butyldiphenylacetamide, m. 201-2°.

N-tert-Amyldiphenylacetamide (76% yield) m. 180°.

IT 20225-93-8P, Isoquinoline,

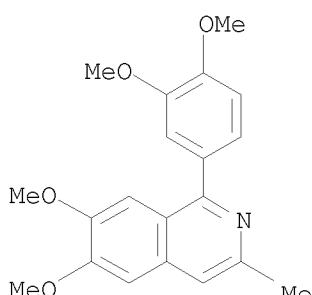
1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl-, hydrochloride

RL: PREP (Preparation)

(preparation of)

RN 20225-93-8 HCAPLUS

CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

L13 ANSWER 270 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1953:19089 HCAPLUS

DOCUMENT NUMBER: 47:19089

ORIGINAL REFERENCE NO.: 47:3315f-i,3316a-f

TITLE: New spasmolytic derivatives of 1-phenylisoquinoline

AUTHOR(S): Tsatsas, Georges

CORPORATE SOURCE: Faculte sci., Paris

SOURCE: Annales Pharmaceutiques Francaises (1952),

10, 276-91

CODEN: APFRAD; ISSN: 0003-4509

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

OTHER SOURCE(S):

CASREACT 47:19089

AB As intermediates were prepared 2,3-(MeO)2C6H3CO2H (I), m. 122°; 2,3-(EtO)2C6H3CO2H (II), m. 59-9.5°; 2,3-(MeO)2C2H3COCl (III); the di-Et analog (IV), b16 152-3°; 3,4-(MeO)2C6H3C2H4NH2 (V), b12 158-60°, prepared in 70% yield by mixing methylvanillin in EtOH with CH₃NO₂ and MeNH₂ in H₂O and AcOH and reducing the nitrostyrolene obtained with Zn-Hg in HCl, or by hydrogenating methylvanillin in the presence of Raney Ni to the alc., b11 166-7° (100%), transforming the latter with HCl in ClCH₂CCl₂ into the chloride, and this with KCN into the cyanide, b14 177-85°, m. 65° (80%), which is reduced with H and Raney Ni; 3,4-(MeO)2C6H3CH(OMe)CH₂NH₂ (VI), prepared from 3,4-(MeO)2C6H3CH:CHNO₂; the di-Et analog (VII) of V; 2,3-(EtO)2C6H3CH(OH)CH₂NH₂ (VIII), prepared from the NO₂ compound (67.2-70%). VIII gives with BzCl and N KOH 05.7% oily 2,8-(EtO)2C6H3CH(OH)CH₂NHBz (IX); VIII and 2,3-(MeO)2C3H3COCl (X) in Et₂O in the presence of KOH give 2,3-(EtO)C6H3CH(OH)CH₂NHCOC₆H₃-(OMe)2-2,3 (XI) (96.5%); VIII and 2,3-(EtO)2C6H3COCl give the oily di-Et analog (XII) of XI (95.6%). 2,3-(MeO)2C6H3-CH(OMe)CH₂NH₂ (XIII) gives with X in EtOH and KOH 94.3% 2,3-(MeO)2C6H3CH(OMe)CH₂NHOCC₆H₃(OMe)2-2,3 (XIV), m. 104°. VI gives with X 90.4 % of the corresponding benzamide (XV), m. 119.5°. XIII and BzCl give 96% of the benzamide (XVI), m. 93-3.5°. 2,3-(MeO)2C6H3C2H4-NH₂ (XVII) and BzCl give 92% of the benzamide (XVIII), m. 85.5°. The di-Et analog of XVIII (98.5%) is an oil. Adding X in Et₂O to cold 2,3-(EtO)2C6H3C2H4NH₂ (XIX) in KOH gives 87.8% oily 2,3-(EtO)2C6H3C2H4NHOCC₆H₃-(OMe)2-2,3 (XX), which is also obtained by distillation of XIX with 2,8-(MeO)2C6H3CO₂H and xylene. This reaction is not complete. Distillation of VII and 2,3-(EtO)2C6H3CO₂H with xylene gives 78.6%

of

the benzamide (XXI), m. 67°. XVII and X give in Et₂O with KOH the benzamide (XXII), m. 71° (from MeOH-H₂O) (91.8%). V and X give 95% of the benzamide (XXIII), m. 110-11°. Reflux 15 g. of the Et analog of XVIII 20 min. with 30 cc. POCl₃ in 150 cc. xylene, evaporate in vacuo, dissolve in hot H₂O, shake out with Et₂O, precipitate with NaOH, extract with

Et₂O, and evaporate, obtaining 98.5% 1-phenyl-3,4-dihydro-5,6-diethoxyisoquinoline (XXIV), m. 94° (from EtOH-H₂O); HCl salt, m. 197° (decomposition), easily soluble in H₂O. Refluxing XXIV in tetrahydronaphthalene with Pd black (10%) 210 min., filtering, extracting with HCl, and precipitating with NaOH gives 100% 1-phenyl-5,6-diethoxyisoquinoline, m.

63° (from C₆H₆-petr. ether); HCl salt, m. 183°, decompose 140° on gradual heating, soluble in H₂O, EtOH, Me₂CO, also prepared by refluxing IX 20 min. in xylene with POCl₃, evaporating, dissolving in H₂O, precipitating with NaOH, and purifying by chromatography on Al₂O₃. Refluxing XVIII with POCl₃ in xylene gives 95.1%

1-phenyl-3,4-dihydro-5,6-dimethoxyisoquinoline, m. 102° (from C₆H₆-petr. other); HCl salt, m. 208°, soluble in H₂O, EtOH, insol. in Me₂CO. Reducing the preceding base with Pd black (10%) in tetrahydronaphthalene gives 1-phenyl-5,6-dimethoxyisoquinoline, m. 107.5-8°, also prepared by heating XVI with POCl₃ in xylene (59.5%); HCl salt, m. 201°, decompose on gradual heating at 160°, soluble in H₂O and EtOH. Heating XXIII with POCl₃ in xylene gives 95.6% 1-(2,3-dimethoxyphenyl)-3,4-dihydro-6,7-dimethoxyisoquinoline, m. 129.5-30° (from C₆H₆-petr. ether); HCl salt, m. 202°, easily

STN

soluble in H₂O, EtOH, and Me₂CO. Reduction with Pd in tetrahydro-naphthalene gives 100% 1-(2,3-dimethoxyphenyl)-6,7-di-methoxyisoquinoline, m. 137° (from C₆H₆-petr. ether), also obtained in 66.6% yield from XV with POCl₃ in xylene; HCl salt, m. 206°, decompose 160° on gradual heating, soluble in H₂O and EtOH, sparingly in Me₂CO. XXII gives with POCl₃ in xylene 97.7% 1-(2,3-dimethoxyphenyl)-3,4-dihydro-5,6-di-methoxyisoquinoline, m. 104° (from C₆H₆-petr. ether). Treatment with Pd in tetrahydronaphthalene gives 80% 1-(2,3-dimethoxyphenyl)-5,6-dimethoxyisoquinoline, m. 86.5° after purification by chromatography, also obtained from XIV with POCl₃ (64.1%); HCl salt, m. 204° (decomposition), soluble in H₂O, EtOH, and Me₂CO.

Distillation

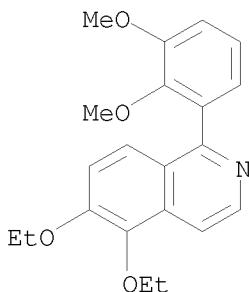
of XX with POCl₃ in xylene gives 52.6-4.7% 1-(2,3-dimethoxy-phenyl)-3,4-dihydro-5,6-diethoxyisoquinoline, m. 92° (from C₆H₆-petr. ether); refluxing with Pd in tetrahydronaphthalene gives 100% 1-(2,3-dimethoxyphenyl)-5,6-diethoxyisoquinoline, m. 87°, also obtained from XI with POCl₃ (36.3%); HCl salt, m. 178° (decomposition), soluble in H₂O, EtOH, and Me₂CO. Refluxing XXI with POCl₃ in xylene gives 83.8% 1-(2,3-diethoxyphenyl)-3,4-dihydro-5,6-diethoxyisoquinoline, m. 159°, which with Pd gives oily 1-(2,3-diethoxyphenyl)-5,6-diethoxyisoquinoline, prepared also from XII with POCl₃ (67%); picrate, m. 125° (from MeOH); HCl salt, m. 113° (decomposition), soluble in H₂O, EtOH, and Me₂CO.

IT 855830-55-6P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(New spasmolytic derivatives of 1-phenylisoquinoline)

RN 855830-55-6 HCPLUS

CN Isoquinoline, 1-(2,3-dimethoxyphenyl)-5,6-diethoxy- (CA INDEX NAME)



L13 ANSWER 271 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1953:6725 HCPLUS
DOCUMENT NUMBER: 47:6725
ORIGINAL REFERENCE NO.: 47:1226b-c
TITLE: Antibacterial substances. II. Antibacterial activities of various hydrazides for *Mycobacterium tuberculosis* in vitro
AUTHOR(S): Kametani, Tetsuji; Yamamura, Yuichi; Uchida, Homare
SOURCE: Yakugaku Zasshi (1952), 72, 1093-6
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

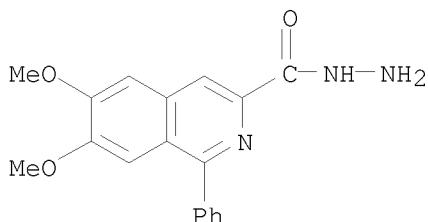
STN

AB cf. C.A. 46, 9657f. Antibacterial action of the following compds. was tested (where R = CONHCH₂CONHNH₂):RR, RCH₂CH₂R, 3,4-(MeO)2C₆H₃R, 3,4-(MeO)2C₆H₃CH(CH₂CONHNH₂)CONHNH₂, PhCONHCH₂CH₂CONHNH₂, p-O₂NC₆H₄R, 3,4-CH₂O₂C₆H₃R, 4- or 3-(I) or 2-RC₅H₄N, 4-RC₉H₆N, and 1-phenyl-6,7-dimethoxyisoquinoline-3-carbohydrazide. The antibacterial action was in the order of heterocyclic compds. > aromatic compds. > aliphatic compds., and I was the strongest among 3 isomers.

IT 860370-71-4, 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-phenyl-, hydrazide
(antibacterial action on Mycobacterium tuberculosis)

RN 860370-71-4 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-phenyl-, hydrazide (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 272 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1953:6391 HCAPLUS
DOCUMENT NUMBER: 47:6391
ORIGINAL REFERENCE NO.: 47:1156a-g
TITLE: Synthesis of 3-hydroxyisoquinolines and 2-hydroxy-1,
4-naphthaquinones from esters of 2-acyl-4,
5-dimethoxyphenylacetic acids
AUTHOR(S): Bentley, H. R.; Dawson, Wm.; Spring, F. S.
CORPORATE SOURCE: Roy. Tech. Coll., Glasgow, UK
SOURCE: Journal of the Chemical Society (1952)
1763-8
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 4, 5-(MeO)2C₆H₃CO₂Et (20 g.) in 120 mL. CS₂, treated with 12 g. AlCl₃ and 6.4 mL. AcCl and refluxed 1 h., gives 51% Et 2-acetyl-4,
5-dimethoxyphenylacetate (I), m. 94° (2, 4-dinitrophenylhydrazone,
red, m. 171°); Me ester (II), m. 114°, 30% (2,
4-dinitrophenylhydrazone, red, m. 194°); hydrolysis of I or II with
5% aqueous KOH gives the acid, m. 175°. Hydrolysis of II with 10% aqueous
NaOH (15 min. at 80°) and the cooled solution treated dropwise (30
min.) with 6 mL. NaOCl and refluxed 15 min. give 2, 4,
5-HO₂C(MeO)2C₆H₂CH₂CO₂H, m. 216°. I (1 g.), shaken 16 h. with 30
mL. NH₄OH (d. 0.88), gives 60% 3-hydroxy-6,
7-dimethoxy-1-methylisoquinoline, yellow, m. 286° (decomposition);
picrate, yellow, m. 236-9°; HCl salt, pale yellow, m. 250°
(decomposition); monoacetate, m. 139-40°. 4, 5-(MeO)2C₆H₃CO₂Me (III)
with BzCl and AlCl₃ in CS₂, refluxed 2 h., gives 34% Me 2-benzoyl-4,

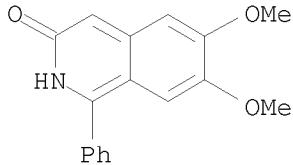
5-dimethoxyphenylacetate (IV), m. 107°; the acid m. 163°. IV (1 g.) and 30 mL. saturated EtOH-NH₃, heated 4 h. at 130-40°, give 61% 3-hydroxy-6, 7-dimethoxy-1-phenylisoquinoline, yellow, m. 243° (decomposition). III (20 g.), 14.8 g. PhCH₂COCl, and 12.8 g. AlCl₃ in 120 mL. CS₂, boiled 1 h., give 32% Me 4, 5-dimethoxy-2-(phenylacetyl)phenylacetate (V), m. 94° (2, 4-dinitrophenylhydrazone, red, m. 148°). 4, 5-(MeO)₂C₆H₃-COCl (7 g.), added to 7 g. AlCl₃ in 50 mL. ice-cold PhNO₂ and the mixture treated dropwise (1 h.) with 10 g. III, with stirring overnight at room temperature, gives 13% Me 4, 5-dimethoxy-2-(3, 4-dimethoxyphenylacetyl)phenylacetate (VI), m. 132° (2, 4-dinitrophenylhydrazone, red, m. 150°). V (200 mg.), shaken 2 days with 10 mL. 5% NaOH or 10 mL. concentrated NH₄OH, gives 53% 2-hydroxy-6, 7-dimethoxy-3-phenyl-1, 4-naphthoquinone (VII), red, m. 255°, red-brown color with EtOH-FeCl₃ and a dark green color with concentrated H₂SO₄; monoacetate, yellow, m. 218-20°; monobenzoate, orange, m. 232°; VII and CH₂N₂ in ether give the 2,6,7-tri-MeO analog, yellow, m. 214°. Reductive acetylation of VII gives 60% 1,2,4-triacetoxy-6, 7-dimethoxy-3-phenylnaphthalene, m. 175-7°. VI with NaOH or NH₄OH gives 2-hydroxy-6, 7-dimethoxy-3-(3, 4-dimethoxyphenyl)-1, 4-naphthoquinone, red, m. 226°; monobenzoate, orange, m. 206°. 3, 4-Dihydro-6, 7-dimethoxy-1(2H)-naphthalenone (5.2 g.), 7.5 g. p-O₂NC₆H₄NMe₂ in 150 mL. EtOH, and 5 mL. 10% NaOH, kept overnight at room temperature, give 46% 1,2,3,4-tetrahydro-1-oxo-6, 7-dimethoxy-2, 4-bis(p-dimethylanilo)naphthalene (VIII), KMnO₄ color, m. 230° (decomposition); 10 g. VIII and 300 mL. 20% H₂SO₄, refluxed 1 h., give 16% 2-hydroxy-6, 7-dimethoxy-1, 4-naphthoquinone (IX), orange, m. 212° (decomposition). I (1 g.) in 30 mL. EtOH and 0.18 g. Na in 5 mL. EtOH, refluxed 20 min. and kept overnight at room temperature with free access to air, give 80% IX. IX (560 mg.) and PhN₂Cl give 50 mg. VII.

IT 89721-03-9P, 3-Isoquinolinol, 6,7-dimethoxy-1-phenyl-

RL: PREP (Preparation)
(preparation of)

RN 89721-03-9 HCPLUS

CN 3(2H)-Isoquinolinone, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L13 ANSWER 273 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1952:67068 HCPLUS
DOCUMENT NUMBER: 46:67068
ORIGINAL REFERENCE NO.: 46:11208e-h
TITLE: Syntheses of isoquinoline derivatives. XVI. Synthesis of 1-phenyl-3-veratryl-6,7-dimethoxyisoquinoline
AUTHOR(S): Kametani, Tetsuji

STN

CORPORATE SOURCE:

Univ. Osaka

SOURCE:

Yakugaku Zasshi (1952), 72, 85-7

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

AB Catalytic reduction of 20 g. 3,4-(MeO)2C6H3CH:CHCOC6H3(OMe)2-3',4' in 350 ml. AcOEt 5 hrs. with 0.2 g. PdCl₂ and 1.8 g. C, and recrystn. from alc. gives 3,4-(MeO)2C6H3(CH₂)2COC6H3(OMe)2-3',4' (I), m. 88°. EtONa (0.4 g. Na and 10 ml. absolute alc.), 2.1 g. I in 15 ml. C₆H₆ and 20 ml. alc., and 3 g. AmNO₂ heated on a water bath 2 hrs., the solvents removed, water added, the solution extracted with ether, and the mother liquor agitated with

10%

HCl gives 2 g. 3,4-(MeO)2C6H3CH₂C(:NOH)COC6H3(OMe)2-3',4' (II), m. 107-8°. II (4.6 g.) in 200 ml. alc. on catalytic reduction with 0.2 g. PtO₂ and 6.5 ml. HCl for 1 day and further addition of 0.2 g. PdCl₂, absorbed 1070 ml. H₂; the mixture filtered, the alc. removed, HCl added, the solution extracted with ether, and the HCl solution made alkaline with NaOH and extracted with ether gave 4.1 g. (92%) 3,4-(MeO)2C6H3CH₂CH(NH₂)CH(OH)C6H3(OMe)2-3',4' (III), b₂₃ 127°; 2.9 g. III in 20 ml. 10% NaOH treated with 2 g. BzCl in C₆H₆ dropwise with cooling gave 3.5 g. (93%) N-Bz derivative (IV), m. 127°; 0.5 g. IV in 10 ml. C₆H₆ and 5 g. POCl₃ heated on a water bath 2 hrs., petr.-ether added, the mixture let stand overnight, the upper layer decanted off, 10% HCl added, and the solution precipitated with 10% NaOH gave

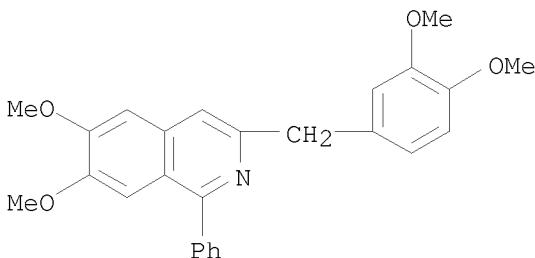
0.3 g. 1-phenyl-3 - veratryl - 6,7 - dimethoxyisoquinoline (V), m. 184-5°; picrate, decompose 220°. The reaction in PhMe gives a product (VI), decompose 95°, beside V; VI may have been derived from V by the migration of double bond to give 1-phenyl - 3 - veratrylidene - 3,4 - dihydro - 6,7 - dimethoxyisoquinoline, and the possibility of such transition is being investigated.

IT 855650-05-4P, Isoquinoline, 6,7-dimethoxy-1-phenyl-3-veratryl-
RL: PREP (Preparation)

(preparation of)

RN 855650-05-4 HCPLUS

CN Isoquinoline, 3-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 274 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1952:26671 HCPLUS

DOCUMENT NUMBER: 46:26671

ORIGINAL REFERENCE NO.: 46:4547h-i, 4548a-c

TITLE: Syntheses of aminoisoquinoline derivatives. II. A

synthesis of 1-phenyl-3,4-dihydro-4-amino-6,7-dimethoxyisoquinoline derivatives

AUTHOR(S):

Kametani, Tetsuji

CORPORATE SOURCE:

Tokyo Coll. Pharmacy

SOURCE:

Yakugaku Zasshi (1951), 71, 332-5

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

GI For diagram(s), see printed CA Issue.

AB Esterification of 15 g. 3,4-(MeO)2C6H3CH(CO2H)CH2CO2H and 60 ml. EtOH with 15 ml. 33% HCl 3 hrs. on the water bath, removal of the EtOH, taking up with ether, washing with alkali and H₂O, and distilling yielded 75% 3,4-(MeO)2C6H3CH(CO2Et)CH2CO2Et (V), b₆ 200-1°. Boiling 10 g. V in 20 ml. alc. with 10 g. H₂NNHOH 7 hrs. and letting stand overnight gives 8 g. 3,4-(MeO)2C6H3CH(CONHNH₂)CH2CONHNH₂ (VI), needles, m. 170-1°. Treating 3 g. VI in 12 ml. 10% HCl and C₆H₆ dropwise with 2.2 g. NaNO₂ in H₂O, decanting off the C₆H₆, extracting the aqueous layer several times with C₆H₆,

combining the exts., treating with 3.3 g. PhCH₂OH, evaporating off the C₆H₆, steam-distilling to remove the PhCH₂OH, and recrysg. the residue from alc. gives 2.2 g. 3,4-(MeO)2C6H3CH(NHCO₂CH₂Ph)CH₂NHCO₂CH₂Ph (VII), m. 67-9°; the mother liquor from VII with H₂O gives 3,4-(MeO)2C6H3CH.N(CO₂CH₂Ph).CO.NH.CH₂ (VIII), m. 137°. Heating VII in 30 ml. (1:1) 20% HCl and glacial AcOH 1.5 hrs. over a direct flame gives a brown liquid; distilling this in vacuo gives a resinous substance (IX) and a yellow powder of the HCl salt of 3,4-(MeO)2C6H3CH(NH₂)CH₂NH₂, which when taken up in H₂O, filtered, alkalinized, treated with 1 g. BzCl, alkalinized, let stand overnight, and filtered gives 1 g. 3,4-(MeO)2C6H3CH(NHBz)CH₂NHBz (X), m. 200-2°. X (0.7 g.) and 1.5 g. POCl₃ in 10 ml. C₆H₆ heated 4 hrs. on the water bath, treated with petr.-ether as before, let stand overnight, the solvent removed, the residue taken up with alc. HCl, filtered, made alkaline with NH₄OH, filtered, and the precipitate washed with

H₂O

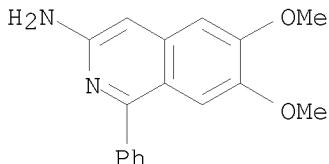
gives 0.4 g. 1-phenyl-3,4-dihydro-4-benzamido-6,7-dimethoxyisoquinoline (XI), m. 155-7°; XI.H₂PtCl₆, decompose 167°. X (1.1 g.) and 1.4 g. POCl₃ in 35 ml. PhMe heated 4 hrs. at 125-32°, treated with petr.ether, taken up with 10% HCl, made alkaline with NH₄OH, and taken up with ether gives 0.9 g. XI.

IT 875249-30-2P, Isoquinoline, 3-amino-6,7-dimethoxy-1-phenyl-

RL: PREP (Preparation)
(preparation of)

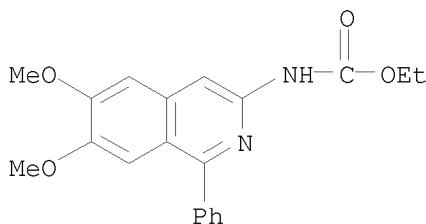
RN 875249-30-2 HCAPLUS

CN 3-Isoquinolinamine, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)



STN

DOCUMENT NUMBER: 46:26670
ORIGINAL REFERENCE NO.: 46:4547f-h
TITLE: Syntheses of aminoisoquinoline derivatives. I.
Saponification of benzyl
1-phenyl-6,7-dimethoxy-3-isoquinolyl carbonate
AUTHOR(S): Kametani, Tetsuji
CORPORATE SOURCE: Tokyo Coll. Pharmacy
SOURCE: Yakugaku Zasshi (1951), 71, 329-31
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Et 1-phenyl-6,7-dimethoxy-3,4-dihydro-3-isoquinolinecarboxylate (I) (2 g.)
in 10 ml. glacial AcOH and 20 ml. 10% HCl treated with 0.5 g. KMnO4 (saturated
solution), heated at 50-60°, filtered, alkalinized with NH4OH, taken
up with AcOEt, dried with Na2SO4, and the residue recrystd. 3 times from
MeOH gives 1.04 g. 1,6,7,3-Ph(MeO)2C9H3NCO2Et (II), needles, m.
168-70°; hydrazide (IIA), m. 217°, Me ester of II, m.
172-3°; benzyl ester (III) of IIA needles, m. 126° (picrate,
needles, m. 183-4°). Saponifying 1 g. III in 5 ml. 20% HCl and 5 ml.
glacial AcOH by heating 1 hr. over a direct flame, distilling with steam,
evaporating to dryness, taking up with H2O, filtering with C, alkalinizing with
NH4OH, taking up with ether, and recrystg. from alc. gives
1,6,7,3-Ph(MeO)2(H2N)C9H3N (IV), decompose 214°, also prepared by the
catalytic reduction of III with Pd-C.
IT 855691-15-5, 3-Isoquinolinecarbamic acid,
6,7-dimethoxy-1-phenyl-
RL: PREP (Preparation)
(derivs.)
RN 855691-15-5 HCPLUS
CN 3-Isoquinolinecarbamic acid, 6,7-dimethoxy-1-phenyl-, ethyl ester (5CI)
(CA INDEX NAME)



L13 ANSWER 276 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1952:21264 HCPLUS
DOCUMENT NUMBER: 46:21264
ORIGINAL REFERENCE NO.: 46:3656h-i
TITLE: Relation between structure and spasmolytic quantities
of some isoquinoline derivatives. II. Substituted
phenylisoquinolines
AUTHOR(S): Tsatsas, Georges; Fournel, Julien
CORPORATE SOURCE: Usines Rhone-Poulenc, Paris
SOURCE: Annales Pharmaceutiques Francaises (1951),
9, 585-92
CODEN: APFRAD; ISSN: 0003-4509

STN

DOCUMENT TYPE:

Journal

LANGUAGE:

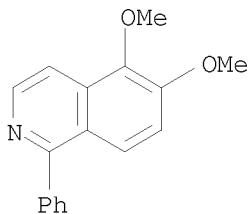
Unavailable

AB cf. C.A. 46, 1160f. The HCl salts of the following isoquinoline derivs. were studied: 1-phenyl-5,6-dimethoxy, 1-phenyl-5,6-diethoxy, 1-(2,3-dimethoxyphenyl)-5,6-dimethoxy, 1-(2,3-dimethoxyphenyl)-5,6-diethoxy, 1-(2,3-diethoxyphenyl)-5,6-diethoxy. The products are of low toxicity, weakly anesthetic, and have no analgesic action. The antispasmodic action is inferior to that of papaverine and perparine.

IT 108974-42-1, Isoquinoline, 5,6-dimethoxy-1-phenyl-
(spasmolytic action of)

RN 108974-42-1 HCPLUS

CN Isoquinoline, 5,6-dimethoxy-1-phenyl- (CA INDEX NAME)



L13 ANSWER 277 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1952:17631 HCPLUS

DOCUMENT NUMBER: 46:17631

ORIGINAL REFERENCE NO.: 46:3056b-g

TITLE: Benzylisoquinoline. II

AUTHOR(S): Shapiro, David

CORPORATE SOURCE: Weizmann Inst. Sci., Rehovoth, Israel

SOURCE: Journal of Organic Chemistry (1951), 84,
1247-9

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 46:17631

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 45, 2945i. 4-Benzylisoquinoline derivs. are prepared for pharmacol. tests. Adding 13 g. RCH₂CR.CH₂.NH.CO.O (R = 3,4-(MeO)₂C₆H₃ throughout the abstract) in small portions to 30 cc. concentrated HCl, heating the

mixture 0.5 hr. on a water bath, neutralizing the chilled solution with K₂CO₃, making it alkaline with NaOH, and extracting with ether and C₆H₆ give 8 g. 2,3-bis(3,4-dimethoxyphenyl)-2-hydroxypropylamine, RCH₂CR(OH)CH₂NH₂ (I), m. 112° (HCl salt, m. 220°). Heating 1.2 g. I with 1.2 g.

KHSO₄ 10 min. at 150°/10 mm., taking up the melt in C₆H₆ and H₂O, making the aqueous layer alkaline and extracting with C₆H₆ give

2,3-bis(3,4-dimethoxyphenyl)allylamine, RCH:CRCH₂NH₂ (II), m. 103° (HCl salt, m. 260-2°), which, hydrogenated in MeOH in the presence of Raney Ni, gives RCH₂CHRCH₂NH₂ (III). Refluxing 4 g. I.HCl in 40 cc. HCO₂H 5 hrs., evaporating the mixture to dryness, and recrystg. the residue

give

II.HCl. Adding 23 g. RCHO and 0.3 g. NH₂Na to 23 g. RCH₂CN in 100 cc.

STN

EtOH and refluxing the mixture 5 min. give 37 g. RCH:CRCN (IV), m. 155°. Hydrogenating 23 g. IV in 200 cc. MeOH and 75 cc. 20% NH₃-MeOH 4 hrs. in the presence of Raney Ni at 100° and 500 lb., evaporating the filtered solution in vacuo, dissolving the residue in 100 cc.

5%

HCl, making the washed (C₆H₆) acid solution alkaline, and extracting with C₆H₆ give

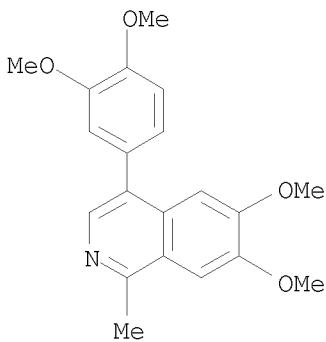
19.5 g. III, b0.4 225-7°, m. 88-9° (HCl salt, m. 223°). III (6.6 g.) in 30 cc. CHCl₃ and 1.6 cc. C₅H₅N with 1.6 g. AcCl in 15 cc. CHCl₃ at 8-10° give 7.3 g. N-Ac derivative (V), b0.3 255°, m. 110-12°. Heating 2.5 g. V and 7.5 g. POCl₃ in 15 cc. xylene 1 hr. at 100°, treating the washed yellow cake with concentrated NaOH, and extracting with C₆H₆-ether give 2.1 g. 4-(3,4-dimethoxyphenyl)-1-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline (VI), b0.3 242-4°, m. 123-4° (HCl salt, m. 187°). Heating 1 g. VI in a CO₂ atmospheric with 0.2 g. 10% Pd-charcoal gives 0.8 g. 4-(3,4-dimethoxyphenyl)-1-methyl-6,7-dimethoxyisoquinoline (VII), b0.15 230-5°, m. 147-9° (HCl salt, m. 210-11°). Whereas VI, in doses of 25 mg./kg. mouse, and VII, 50 mg./kg., administered intraperitoneally, are toxic, all other compds. are neg. in analgesic tests.

IT 102012-78-2P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Benzylisoquinoline. II)

RN 102012-78-2 HCPLUS

CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L13 ANSWER 278 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1952:8571 HCPLUS

DOCUMENT NUMBER: 46:8571

ORIGINAL REFERENCE NO.: 46:1528e-i,1529a-h

TITLE: Dimeric propenyl phenol ethers. XII. The synthetic stereoisomer of diisohomogenol, diisoeugenol diethyl ether, and metanethole

AUTHOR(S): Muller, Alexander; Toldy, Lajos; Halmi, Gabor;

CORPORATE SOURCE: Meszaros, Miomir
 SOURCE: Univ. Budapest, Hung.
 Journal of Organic Chemistry (1951), 16,
 481-91
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB cf. C.A. 42, 3386a; 44, 3477c. 1-(3,4-Dimethoxyphenyl)-2-methyl-5,6-dimethoxy- Δ^1 -inden-3-one (8 g.) in 150 cc. warm anhydrous dioxane is added to EtMgBr from 8 g. EtBr in 70 cc. ether, the mixture is refluxed 40 min., decomposed with ice-H₂O containing 10 g. NH₄Cl, extracted with ether, and the extract evaporated, giving 18% 1-(3,4-dimethoxyphenyl)-2-methyl-3-ethyl-5,6-dimethoxy- Δ^1 -inden-3-ol, needles, m. 128°. When the Grignard complex is dissolved in 120 cc. EtOH and hydrogenated at atmospheric pressure in the presence of 0.6 g. 10% Pd-charcoal 4 h., 31% β -form of 1-(3,4-dimethoxyphenyl)-2-methyl-3-ethyl-5,6-dimethoxyindan (I), long needles, m. 105-6°, is obtained. I gives a purple-violet color in AcOH with Br. Refluxing I in MeOH containing 1% HCl leaves it unchanged. Adding dropwise 10 cc. 10% Br in ether to 0.2 g. I in 10 cc. ether, keeping the mixture 0.5 h. at 25°, and washing the solution with 10% NaHSO₃ give 0.18 g. 1-[3,4,6-(MeO)₂BrC₆H₄] analog, stout prisms, m. 125-6°, mixed with bromodiisohomogenol (m. 126°) m. 102-5°. Refluxing 7.5 g. 3,4-(MeO)(OH)C₆H₃CH₂OEt, 5.6 g. (EtCO)₂O, and 3.7 g. NaOAc 24 h. at 180-90°, extracting the warm mixture with 10% Na₂CO₃, and acidifying the aqueous filtrate give 3.4 g. 3-methoxy-4-ethoxy- α -methylcinnamic acid (II), needles, m. 131-2°. Refluxing with stirring 3 g. II in 30 cc. H₂O and 15 cc. concentrated H₂SO₄ gives 2.2 g. diisoeugenol di-Et ether [α -form of 1-(3-methoxy-4-ethoxyphenyl)-2-methyl-3-ethyl-5-methoxy-6-ethoxy-indan] (III), fibrous needles, m. 130°, which is also formed on ethylation of diisoeugenol (m. 180-1°) with EtBr and alkali. Adding 133 g. Na₂Cr₂O₇ in 60 cc. H₂O, 260 cc. AcOH, and 21 cc. concentrated H₂SO₄ to 80 g.

III (cf. Puxeddu and Rattu, C.A. 31, 3463.8) in 400 cc. AcOH at 25° over a period of 1 h., stirring the mixture 6 h., keeping it 2 days, pouring it into 4 l. H₂O, and extracting with C₆H₆ give 52 g. 1-[6-(3-methoxy-4-ethoxybenzoyl)-3-methoxy-4-ethoxyphenyl] Pr Me ketone (IV), spheroids, m. 148°; IV is not changed when treated with Ac₂O-C₅H₅N. Treating 2 g. IV in 5 cc. C₅H₅N with 0.4 g. HONH₂.HCl 0.5 h. at 100° gives 0.8 g. 1-(3-methoxy-4-ethoxyphenyl)-3-methyl-4-ethyl-6-methoxy-7-ethoxyisoquinoline 2-oxide, crystalline powder, m. 143-4°. Warming 1.15 g. IV in 30 cc. EtOH with 15 cc. 20% aqueous NaOH 10 min. at 100°, diluting the mixture with H₂O, and acidifying with 3 cc. concentrated HCl give 1.2 g. 1-(3-methoxy-4-ethoxyphenyl)-4-ethyl-6-methoxy-7-ethoxy-3-naphthol, slightly colored plates, m. 143° (picrate, brown-violet needles, m. 143-4°). Heating 31 g. IV in 30 cc. AcOH and 10 cc. concentrated H₂SO₄ on a water bath 10 min. with dropwise addition of 100 cc. EtOAc gives 28 g. 1-(3-methoxy-4-ethoxyphenyl)-3-methyl-4-ethyl-6-methoxy-7-ethoxyisobenzopyrylium-H₂SO₄ (V), golden-yellow needles, m. 227-8°. Warming 0.75 g. V in 30 cc. H₂O 2 h. on a water bath give 0.39 g. IV. Dropwise addition of 10% HNO₃ to a 5% solution of V in H₂O gives the nitrate, clusters of bright yellow silky needles, m. 123°. Adding dropwise 25 g. KMnO₄ in 600 cc. H₂O to 20 g. V in 300 cc. H₂O at 25° with

stirring until a crimson color remains for 10 min., dissolving the MnO₂ by dropwise addition of 40% NaHSO₃, shaking the filtered precipitate with 150 cc.

C₆H₆

and 100 cc. 5% HCl, and evaporating the washed (10% Na₂CO₃) C₆H₆, solution give 2.4-3.2 g. of a compound (VI), m. 125-40°. Acidification of the Na₂CO₃ washings give 3,4-(MeO)(EtO)C₆H₃CO₂H, m. 193°. Warming 8 g.

VI with 30 cc. EtOAc containing 10% HCl gently on a water bath and adding 30 cc. EtOH to the cooled mixture give 4.5 g.

1-(3-methoxy-4-ethoxyphenyl)-2-methyl-5-methoxy-6-ethoxy-Δ1-inden-3-one (VII), thin red needles, m. 132-3°, which is also obtained in 2.05-g. yield when 4 g. VI is warmed with 50 cc. 5% NaOH-MeOH 10 min. (phenylhydrazone, bright orange prisms, m. 188°). Treating 3.5 g.

VII in 60 cc. AcOH with 2.3 g. CrO₃ in 5 cc. H₂O and 40 cc. AcOH 10 min. at 25°, warming the mixture 15 min. on the water bath, diluting with 300 cc. H₂O, and extracting with C₆H₆ give 2.6 g.

6-(acetylcarbonyl)-3',4-dimethoxy-3,4'-diethoxybenzophenone (VIII), long yellow lancets, m. 173-4° (quinoxaline derivative, golden-yellow silky needles, m. 217-19°). Adding 5 cc. 20% H₂O₂ to 0.5 g. VIII in 100 cc. 20% NaOH, shaking the mixture until all is dissolved, and acidifying it give 0.36 g. 2-(3-methoxy-4-ethoxyphenyl)-4-ethoxy-5-methoxybenzoic acid, stout prisms, m. 215°. Adding 8 g. VII in 120 cc. warm anhydrous dioxane to EtMgBr from 8 g. EtBr in 70 cc. ether, refluxing the mixture 1 h., decomposing it with iced NH₄Cl, extracting with ether, and hydrogenating

the

residue of the washed and dried ether extract in EtOH with Pd-charcoal gives 3.2 g. β-form of 1-(3-methoxy-4-ethoxyphenyl)-2-methyl-3-ethyl-5-methoxy-6-ethoxyindan (IX), slender prisms, m. 115.5°. IX gives a purple-violet color with Br in AcOH. Oxidation of 0.5 g. IX with Na₂Cr₂O₇ gives 0.2 g. IV, plates, m. 147-8°. Treating 0.5 g. IX in 50 cc. ether with 0.1 cc. Br in 30 cc. ether 0.5 h. at 25° and washing the solution with 5% NaHSO₃ give the 6-Br derivative, plates, m. 111°. Adding 2 g. finely powdered 1-p-anisyl-2-methyl-6-methoxy-Δ1-indenone to Et-MgBr from 1.6 g. EtBr in 25 cc. ether, pouring the solution immediately into ice-cold 1% NH₄Cl, extracting it with ether, evaporating the washed

(NH₄Cl,

H₂O) ether solution, and hydrogenating the residue in EtOH in the presence of 5% Pd-charcoal 1.5 h. give 57% β-form of

1-p-anisyl-2-methyl-3-ethyl-6-methoxyindan (X), long needles, 100-1°. X is also obtained when 18 g.

2-methyl-3-ethyl-6-methoxyindanone [prepared according to the method of van der Zanden and de Vries (C.A. 43, 6608c)] in 100 cc. ether is added to p-MeOC₆H₄MgBr from 37.4 g. bromide in 200 cc. ether, the mixture is kept 10 min., poured into ice-cold 2% HCl, extracted with AcOEt, and the residue of the washed (1% HCl) extract is distilled, giving a pale yellow oil, b0.01 160-70°, which, dissolved in 100 cc. EtOH, gives 0.9 g.

p,p'-dianisyl, m. 174-6°. From the mother liquor 27%

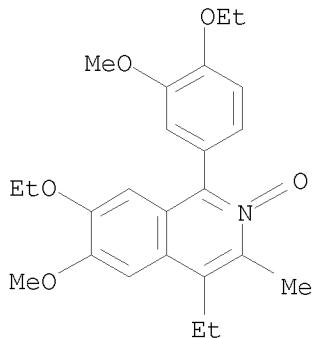
1-p-anisyl-2-methyl-3-ethyl-6-methoxy-Δ1-indene (XI), slender needles, m. 67-8°, is obtained. Hydrogenating 5 g. XI in Et OH with Pd-charcoal 10 h. gives 4 g. X. X gives no color with Br in AcOH and no precipitate with concentrated HNO₃. Treating 0.2 g. X with Br in AcOH gives a

mono-Br derivative, C₂₀H₂₈BrO₂, small needles, m. 90-2°. From the mother liquor a 1:4 mixture of mono- and di-Br derivs., prisms, m. 143-6°, is isolated.

IT 855651-31-9P, Isoquinoline,

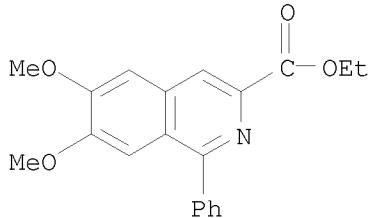
7-ethoxy-1-(4-ethoxy-3-methoxyphenyl)-4-ethyl-6-methoxy-3-methyl-, 2-oxide

RL: PREP (Preparation)
 (preparation of)
 RN 855651-31-9 HCPLUS
 CN Isoquinoline, 7-ethoxy-1-(4-ethoxy-3-methoxyphenyl)-4-ethyl-6-methoxy-3-methyl-, 2-oxide (CA INDEX NAME)



L13 ANSWER 279 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1952:626 HCPLUS
 DOCUMENT NUMBER: 46:626
 ORIGINAL REFERENCE NO.: 46:115f-i,116a
 TITLE: Synthesis of aminoisoquinolines. I. Synthesis of 1-phenyl-3-amino-6,7-dimethoxyisoquinoline
 AUTHOR(S): Hosono, Takeshi
 CORPORATE SOURCE: Tokyo Coll. Pharm.
 SOURCE: Yakugaku Zasshi (1945), 65(No. 7/8A), 11
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Many compds. with an NH₂ group in the aromatic nucleus at the 1-position of 1-phenylisoquinoline derivs. are known as intermediate products of aporphine-type bases, but no study has been made of the physiol. action of these amino compds. Morimoto (cf. preceding abstract) prepared 1-(aminophenyl)-3-methyl-6,7-methylenedioxyisoquinoline and their ureido and sulfonamido derivs. to test their physiol. actions. Since there are few compds. with an NH₂ group in the isoquinoline nucleus the synthesis of such compds. was undertaken. 1-Phenyl-3-amino-6,7-dimethoxyisoquinoline (I) was derived from the azlactone obtained from veratraldehyde and hippuric acid. The lactone was converted to Et α-veratrylidene hippurate (II) by alc. decomposition of the Na salt and II catalytically reduced by Adams Pt catalyst to 3,4-(MeO)2C₆H₃CH₂CH(NH₂)CO₂Et (III) (Harwood and Johnson, C.A. 28, 1703.3), which yielded Et 1-phenyl-6,7-dimethoxy-3,4-dihydro-3-isoquinolinecarboxylate (IV) (picrolonate, decompose 193°) when boiled a short time with a small amount of POCl₃, but Et 1-phenyl-6,7-dimethoxy-3-isoquinoline-3-carboxylate (V), m. 170°, by self-dehydrogenation on boiling for a long time. IV gave V by heating at 170-180° with Pd black in the presence of cinnamic acid. V gave Et 1-phenyl-6,7-dimethoxy-3-isoquinolylcarbamate (VI), m. 142°, through the corresponding hydrazide, m. 215-16°, and azide (VII), m. (crude) 121-2°. VII was converted to I, yellow crystals, m. 215°, by boiling with 3% alc.

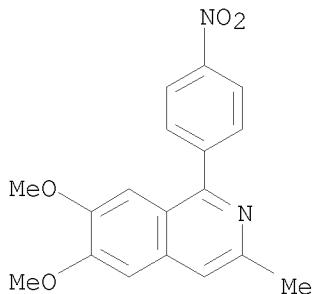
KOH and then heating with weak HCl.
 IT 89242-43-3P
 RL: SPN (Synthetic preparation); PRP (Properties); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (Synthesis of aminoisoquinolines. I. Synthesis of 1-phenyl-3-amino-6,7-dimethoxyisoquinoline)
 RN 89242-43-3 HCPLUS
 CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-phenyl-, ethyl ester (CA INDEX NAME)



L13 ANSWER 280 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1952:625 HCPLUS
 DOCUMENT NUMBER: 46:625
 ORIGINAL REFERENCE NO.: 46:115c-f
 TITLE: Synthesis of 1-(aminophenyl)isoquinolines
 AUTHOR(S): Morimoto, Yasuo
 CORPORATE SOURCE: Kiryu Coll. Technol.
 SOURCE: Yakugaku Zasshi (1942), 62, 446-52
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB p-[3,4-(MeO)2C6H3CH(OMe)CHMeNHCO]C6H4NO2 (I), needles, m. 144-4.5°, is prepared by condensation of 3,4-(MeO)2C6H3CH(OMe)CHMeNH2 and p-O2NC6H4COCl. Cyclization of I is effected by heating 12 g. I in 90 mL. PhMe and 33 mL. POC13 30 min. on an oil bath and taking up in petr. ether. The portions of the residue soluble in HCl are combined, cooled, and the crystals NH4OH is added to obtain a free base, and recrystn. from alc. gives 11.5 g. 1-(p-nitrophenyl)-3-methyl-6,7-dimethoxyisoquinoline (II); HCl salt, needles, m. 252° (decomposition); II.MeI, columns, decompose 232-3°. Reduction of II with Zn gives the 1-(p-aminophenyl) analog (III), needles, m. 170-1°; 1-(p-acetamidophenyl) analog (IV), columns, m. 180-1°; 1-(p-carbethoxyaminophenyl) analog (V), needles, m. 149-50°; 1-(p-ureiodophenyl) analog (VI), columns, m. 167-8°. 1-(p-Aminophenyl)-2,3-dimethyl-1,2,3,4-tetra-hydro-6,7-dimethoxyisoquinoline (VII), needles, m. 173-4°, is prepared by catalytic reduction with PtO2 of II.MeCl, plates, decompose 244-5°; 1-(p-acetamidophenyl) analog (VIII), needles, m. 185-6°; 1-(p-carbethoxyaminophenyl) analog (IX), columns, m. 242-3° (decomposition); 1-(p-ureiodophenyl) analog (X), columns, m. 167-8°. The m.ps. of the o- and m-analogs, resp., of these compds., prepared in the same manner are: I, 176-7°, 193-4°; II, 172-3°, 195-6°; III, 147-8°, 175-6°; IV, 209-10°, 247-8°; V, decompose 287-8°, decompose 180-2°; VI, -, 295-6°; VII, 107-8°, 120-1°; VIII, 194-5°,

STN

106-8°; IX, 208-9°, 108-9°; X, 182-3°, -.
IT 1082684-48-7P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Synthesis of 1-(aminophenyl)isoquinolines)
RN 1082684-48-7 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-3-methyl-1-(4-nitrophenyl)-, hydrochloride
(1:1) (CA INDEX NAME)



● HCl

L13 ANSWER 281 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1951:44353 HCAPLUS
DOCUMENT NUMBER: 45:44353
ORIGINAL REFERENCE NO.: 45:7580g-i, 7581a-i, 7582a
TITLE: Synthetic investigations in the isoquinoline series.
II
AUTHOR(S): Dobrowsky, A.
SOURCE: Monatshefte fuer Chemie (1951), 82, 140-55
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB To 134 g. XXIII in 2 l. C₆H₆ was added with stirring 69 g. 3,4-CH₂O₂C₆H₃COCl in 1 l. C₆H₆, the XXIII.HCl filtered off, and the C₆H₆ filtrate concentrated to give 75% R'CH₂CHMeNHCOC₆H₃O₂CH₂-3,4 (XXXIV); 67 g. XXXIV, 25 cc. POC₁₃, and 300 cc. PhMe refluxed 10 min. gave 70% 1-piperonyl-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (XXXV), white crystals, m. 124° (from MeOH); and XXXV gave 40% of the dehydrogenated base (XXXVI), m. 189° (from C₆H₆ or MeOH); HCl salt, m. 169°. XXXVI (20 g.), 40 cc. MeOH, and 10 g. (MeO)₂SO₂ were boiled 4 h., the MeOH distilled, the residue treated with 50 cc. 7% Na₂CO₃, filtered, the filtrate treated with 5 cc. AcOH, the whole shaken with charcoal, filtered, hydrogenated over Pd, filtered, and a 0.5 volume of concentrated HCl added to give a crystalline HCl salt (XXXVII), which, decomposed with aqueous NaOH, extracted with CH₂Cl₂, and the CH₂Cl₂ solution concentrated and diluted with Et₂O gave 65% 1-piperonyl-2,3-dimethyl-6,7-methylenedioxy-1,2,3,4-tetrahydroisoquinoline, m. 143° from PhMe. XXIII and 3,4-(EtO)₂C₆H₃COCl (XXXVIII), b15 195-7°, white crystals, no m.p.

given, gave $\text{RCH}_2\text{CHMeNHCOOC}_6\text{H}_3(\text{OEt})_2$ -3,4 (XXXIX), m. 135° . XXXIX as above gave 1-(3,4-diethoxyphenyl)-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (XL), white crystals, m. 69° , which gave 70% of the dehydrogenated base, m. 96° (from Et₂O-petr. ether); HCl salt (1 H₂O), m. 234° . EtCO₂H (2.5 mols.) and 1 mol. PCl₃ refluxed 1 h. gave 100% EtCOCl (XLI), b. 75 - 82° . XLI (92 g.), o-C₆H₄(OEt)₂, 300 cc. CS₂, and 176 g. AlCl₃ gave 55% 3,4-(EtO)₂C₆H₃COEt (XLII), b₁₅ 195 - 8° . As above, XLII gave 89% of the isonitroso derivative (XLIII), m. 115° (from MeOH), which gave the amine (XLIV), m. 205° ; XLIV and H over Pd gave 3,4-(EtO)₂C₆H₃CH(OH)CHMeNH₂ (XLV), m. 203° (from H₂O). XXXVIII and XLV gave the amide (XLVI), m. 132° (from PhMe), which gave 1-phenyl-3',4',6,7-tetraethoxy-3-methylisoquinoline, white crystals, m. 94° (from Et₂O); HCl salt (1 H₂O), m. 190° . XXIII and BzCl gave 90% of the amide (XLVII), m. 105° (from alc.); which gave 75% 1-phenyl-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (XLV-III), yellow crystals, m. 102° (from 33% MeOH), and 10% of the red-brown 6,7-di-HO compound (XLIX) (caused by cleavage of the methylenedioxy group). XLVIII (120 g.) and 10 g. Pd kept 1 h. at 220° gave 83% of the dehydrogenated base (L), white crystals, m. 138° (from MeOH); HCl salt (1 H₂O), m. 175° (decomposition). XLVIII, as above, gave the methosulfate (LI); LI (126 g.) and 3 g. PtO₂ under 6 atmospheric of H after 3 min. gave 54% of the 2-methyltetrahydro base, m. 111° (from alc.), HOCH₂CH₂SO₃H salt, m. 160° . LI (25 g.) and 45 g. CH₂:CHCH₂Br after 6 h. at 100° gave 26 g. of the quaternary compound (LII), m. 176° (from H₂O). LII (50 g.), 1200 cc. H₂O, and 6 g. PtO₂ under 6 atmospheric of H at 80° gave 8 g. L and 21.4 g. of the corresponding tetrahydro derivative XLIX and (EtO)₂SO₂ gave the di-Et ether (LIII), m. 101° (from 80% MeOH); HCl salt, m. 221° (decomposition). LIII gave a dehydrogenated base, m. 128° ; HCl salt, m. 240° . 1-Norephedrine and BzCl gave the amide (LIV), m. 170° , which (10 g.) in 240 cc. boiling decahydronaphthalene was treated during 1 h. with 60 g. P₂O₅, cooled, hydrolyzed with H₂O, and extracted with Et₂O to give 1.5-2.5 g. 1-phenyl-3-methylisoquinoline (LV), b₁₂ 208 - 12° , m. 90° (from alc.); HCl salt, white needles, m. 228° (from alc.). PhCH(OMe)CHMeNH₂, b₁₅ 111 - 12° , and BzCl gave the amide (LVI), m. 151° (from alc.), which in decahydronaphthalene, as above, gave LV, m. 89 - 90° . 3,4-CH₂O₂C₆H₃CH:CPhCN (135 g.) was hydrogenated over Pd to give 106 g. 3,4-CH₂O₂C₆H₃CH₂CHPhCN (LVII), m. 57° ; LVII and alc. NaOH gave the acid (LVIII), white crystals, m. 124° (from alc.); from which was obtained the NH₄ salt and, by decomposition at 180° , 3,4-CH₂O₂C₆H₃CH₂CHPhCONH₂ (LIX), m. 144° (from alc.); LIX gave 37% of the amine (LX) (no m.p. given), and by the procedures described above, LX gave 3,4-CH₂O₂C₆H₃CH₂CHPhNH₂Bz, m. 177° (from alc.), which in turn, gave 24% 1,3-diphenyl-6,7-methylenedioxy-3,4-dihydroisoquinoline, m. 147° (from alc.). Et₂C(CO₂H)₂ refluxed 1 h. (190°) gave Et₂CHCO₂H (LXI); LXI and XXIII gave 58% of the amide (LXII), m. 120° (from PhMe), converted in the usual manner to 1-isoamyl-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (LXIII), oil, b₁₂ 190° , and LXIII gave 60% of the dehydrogenated base, white crystals, m. 62° (from MeOH-Et₂O); HCl salt (no m.p. given). XXX and Ac₂O gave the N-Ac derivative, oil. 1,3-Dimethyl-6,7-methylenedioxyisoquinoline formed fine, white crystals, m. 146° (from alc.); picrate, m. 227° (decomposition); HCl salt (no m.p. given). XXX (3.3 g.) and HCO₂Et kept 4 h. at 100° , and

distilled gave the N-formyl derivative as an oil which with 10 cc. PhMe and 1 cc.

POCl₃ after 2 h. reflux gave 0.1 g.

3-methyl-6,7-methylenedioxyisoquinoline, m. 170-1° (from Et₂O).

XXIII and PhCH:CHCOCl, b15 162-5°, gave the amide (LXIV), m.

115° (from alc.); LXIV gave

1-styryl-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (LXV), m.

87° (from C₆H₆-petr. ether); HCl salt, intense yellow, m.

151° [hydrate, m. 121° (decomposition)]. LXV gave the

dehydrogenated base, m. 222° (from PhMe); HCl salt, colorless

crystals (no m.p. given). XXIII and PhCH₂CH₂CO₂H at 180° gave the amide, m. 92° (from PhMe), which in turn gave

1-phenethyl-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (LXVI),

white crystals, m. 127° (from absolute alc.); HCl salt, m. 219°.

LXVI could not be dehydrogenated. XXIII and 9-fluorencarboxyl chloride gave the amide, m. 204° (from alc. and then PhMe), from which was obtained in turn 1-(9-fluorenyl)-3-methyl-6,7-methylenedioxy-3,4-

dihydroisoquinoline, (LXVII), m. 160°; HCl salt, m. 281° (from dilute HCl, then alc.). LXVII could not be dehydrogenated. LXVII in

ether oxidized readily in the air, adding 1 atom O and forming colorless crystals, m. 181° (decomposition); HCl salt, m. 246°. XXIII and

3-C₅H₄NCOCl were carried through the various steps without isolating any intermediates to give 1-(3-pyridyl)-3-methyl-6,7-methylenedioxy-3,4-

dihydroisoquinoline (LXVIII), white crystals, m. 138° (from alc.

and C₆H₆); LXVIII gave in poor yield the dehydrogenated base, white

crystals, m. 193°. The relation between chemical structure and

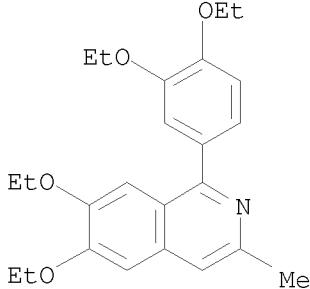
pharmacol. activity is discussed briefly.

IT 873404-59-2P, Isoquinoline,
1-(3,4-diethoxyphenyl)-6,7-diethoxy-3-methyl-

RL: PREP (Preparation)
(preparation of)

RN 873404-59-2 HCPLUS

CN Isoquinoline, 1-(3,4-diethoxyphenyl)-6,7-diethoxy-3-methyl- (CA INDEX
NAME)



L13 ANSWER 282 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1951:44352 HCPLUS

DOCUMENT NUMBER: 45:44352

ORIGINAL REFERENCE NO.: 45:7578i, 7579a-i, 7580a-g

TITLE: Synthetic investigations in the isoquinoline series. I

AUTHOR(S): Dobrowsky, A.

SOURCE: Monatshefte fuer Chemie (1951), 82, 122-39

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB 3,4-Dihydropapaverine (I), large white crystals, m. 102° (from Et₂O), is fairly stable in the solid state; in solution it is easily oxidized to 3,4-dihydropapaveraldine (II), short prisms, m. 195° (from alc.). The hydrated crystalline HCl salt of I. m. about 180° (decomposition). I with Pd-on-C gives II. To 35 g. papaveroline and 600 cc. absolute alc. kept alkaline with alc. NaOH, was added with stirring 114 g. (EtO)₂SO₂ (maximum temperature 40°), the mixture diluted with Et₂O, extracted

with

aqueous NaOH, the Et₂O solution concentrated, and the residue dissolved in a little

petr. ether, giving 13.4 g. tetra-Et ether, m. 102°.

Mescaline-H₂SO₄ 50 g. was decomposed with aqueous NaOH, the free base extracted with

200 cc. C₆H₆, the C₆H₆ solution treated with 41 g. 3,4-(MeO)₂C₆H₃CH₂COCl in

500 cc. C₆H₆, alkali added gradually with cooling and stirring, the precipitated

solid dissolved by warming, and the warm C₆H₆ solution washed with warm aqueous HCl and warm aqueous NaOH, dried with CaCl₂, filtered, and concentrated, giving 100%

of the amide (II), m. 138°. II with POCl₃ in PhMe gave

8-methoxy-3,4-dihydropapaverine (III), prisms, m. 140°, readily dehydrogenated at 160° with Pd. 1-Benzyl-3,4-dihydroisoquinoline (33.4 g.) and 125 g. MeI kept 2 h. at 70° gave the methiodide (IV); IV in MeOH hydrogenated at 60° over Pt gave 26.8 g.

1-benzyl-1,2,3,4-tetrahydro-2-methylisoquinoline, yellow oil, b14

215-18°, picrate, m. 168° (from alc.). 3,4-EtO(MeO)C₆H₃CHO

(V) (73.5 g.) and 42.5 g. CH₂(CO₂H)₂ gave 50 g. hesperitinic acid (VI), m. 176° (23.6 g. V recovered); VI with H and Pd gave the dihydro derivative (VII), m. 104°, converted to the amide (IX), m. 122°,

through the NH₄ salt. IX by the Hofmann procedure gave the amine (X) which with PhCH₂COCl gave 3,4-EtO(MeO)C₆H₃CH₂CH₂NHCOCH₂Ph (XI), m.

103°. XI, as above gave 1-benzyl-6-ethoxy-7-methoxy-3,4-dihydroisoquinoline (XII), m. 61° (from Et₂O-petr. ether), which with Pd gave the dehydrogenated base, m. 127°; HCl salt (1 H₂O), m. 140°. To 23 g. Na in 400 cc. absolute alc. was added 152 g.

3,4-HO(MeO)C₆H₃CHO and 200 g. iso-AmI and the whole refluxed 6 h., giving 57 g. 3,4-iso-AmO(MeO)C₆H₃CHO, b15 186-7°. As above were prepared the following compds. (R = 3,4-iso-AmO(MeO)C₆H₃): RCH:CHCO₂H, m.

172° (from alc.); RCH₂CH₂CO₂H, soft plates, m. 100° (from C₆H₆); RCH₂CH₂CONH₂, m. 114° (from 50% alc.); RCH₂CH₂NH₂, light

oil, b15 192-5°; RCH₂CH₂NHCOCH₂Ph, m. 102° (from alc.);

1-benzyl-6-isoamoxy-7-methoxy-3,4-dihydroisoquinoline (XIII), m.

82°; and the dehydrogenated base (XIV), m. 87°. XIII

considerably depressed the m.p. of XIV. o-C₆H₄(OH)₂ (500 g.) in a hot solution of 260 g. KOH in 300 cc. H₂O refluxed 90 min. with 940 g. (CH₂Br)₂, the whole steam-distilled, and the crude ether in the distillate fractionated gave 36% 1,2-ethylenedioxybenzene (XV), oil, b.

103-5°. XV gave 40% 3,4-(CH₂O)₂C₆H₃CHO (XVI). As above, XVI gave

57% R'CH:CHCO₂H [R' = 3,4-(CH₂O)₂C₆H₃], yellow crystals, m. 182° (from alc.); R'CH₂CH₂CO₂H, white crystals, m. 65°; R'CH₂CH₂CONH₂,

m. 117°; R'CH₂CH₂NH₂, colorless oil, b15 170-3°;

R'CH₂CH₂NHCOCH₂Ph, m. 92°; 1-benzyl-6,7-ethylenedioxy-3,4-dihydroisoquinoline, m. 100° (from C₆H₆-petr. ether); and the

dehydrogenated base (XVII), white crystals, m. 135°. The H₂SO₄ and HCl salt of XVII are difficultly soluble; the MeSO₃H salt is easily H₂O-soluble. From 69 g. 3,4-(EtO)C₆H₃Ac, b15 188-92°, shiny crystals, m. 53° (from Et₂O-petr. ether) in 250 cc. absolute alc., 10 g. Na in 250 cc. absolute alc., and 50 g. AmONO was obtained 16 g. of the isonitroso derivative

(XVIII). The Na salt of XVIII (86 g.), 250 g. SnCl₂, and 250 cc. concentrated HCl gave 31 g. R''COCH₂NH₂.HCl (R'' = 3,4-(EtO)C₆H₃), m. 178°; R''COCH₂NH₂ and H over Pd gave R''CH(OH)CH₂NH₂ [HCl salt, m. 146° (decomposition)]; as above, were obtained R''CH(OH)CH₂NHCOR'', m. 144° (from alc.); 1-phenyl-3',4',6,7-tetraethoxyisoquinoline, m. 107° [HCl salt (1 H₂O), m. 205° (decomposition)]. 3,4-(MeO)C₆H₃CH₂CH.MeNH₂ (XIX) (103 g.) and 106 g. 3,4-(MeO)C₆H₃CH₂CO₂H (XX) were heated 6 h. in an oil bath at 190° while N was passed through the melt, the hot melt dissolved in 1800 cc. PhMe, 130 g. POCl₃ added, and the whole heated 2 h. on a steam bath, giving 57% 3-methyl-3,4-dihydropapaverine (XXI), thick orange syrup; XXI gave 65% 3-methylpapaverine, m. 136° [HCl salt (1 H₂O), m. 90-5°; anhydrous, m. 234°]. XIX and 3,4-(CH₂O)C₆H₃CH₂CO₂H (XXII) as above, gave the amide, m. 110° (from alc.), which gave 1-(3,4-methylenedioxybenzyl)-3-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline, m. 114° (from Et₂O) [HCl salt, m. 144° (from alc.)], and the dehydrogenated base, m. 168-9° (from Et₂O) [HCl salt (1 H₂O), m. 160° (decomposition); anhydrous, m. 233°]. XX and 3,4-(CH₂O)C₆H₃CH₂CHMeNH₂ (XXIII) gave the amide (XXIV), m. 123° (from alc.) which gave 1-(3,4-dimethoxybenzyl)-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (XXV), orange oil, and XXV with Pd gave 80% of the dehydrogenated base, m. 125° (from Et₂O) (HCl salt, m. 220°). XXIII and XXII in decahydronaphthalene gave the amide (XXVI), m. 128° (from alc.), which yielded 1-(3,4-methylenedioxybenzyl)-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline (XXVII), oil (HCl salt, m. 237°); and XXVII gave the dehydrogenated base (XXVIII), white needles, m. 140° (from MeOH) [HCl salt (1 H₂O), m. 160°; anhydrous, m. 255°; tartrate, m. 118°]. 3,4-CH₂O₂C₆H₃CH(OH)CHMeNO₂, b15 208-13° (23.4 g.), and 3.8 g. Na in 100 cc. MeOH kept several hours, the whole made acid with AcOH, concentrated in vacuo, the residue distributed between Et₂O and H₂O, and the Et₂O layer concentrated and distilled, gave 68%

3,4-CH₂O₂C₆H₃CH(OMe)CHMeNO₂

(XXIX), b13 185-90°. XXIX (18 g.) in 90 cc. 85% HCO₂H was treated, with cooling, with 36 g. Cu-activated Zn dust, the whole kept 1.5 h. at 55-60°, filtered, the filtrate concentrated in vacuo, the residue dissolved in H₂O, the solution made alkaline, extracted with Et₂O, the Et₂O solution

extracted with HCl, and the HCl solution made alkaline and extracted with Et₂O, giving

57% of the amine (XXX), colorless, viscous oil, b12 160-5°. XXX (2 mols.) and 3,4-CH₂O₂C₆H₃CH₂COCl 1 mol. in C₆H₆ kept 24 h., filtered from the XXX.HCl, the C₆H₆ solution concentrated, and the residue recrystd. from alc.

gave 3,4-CH₂O₂C₆H₃CH(OMe)CHMeNHCOCH₂C₆H₃O₂CH₂-3,4 (XXXI), white crystals, m. 150°. XXXI gave 64% XXVIII. XX (1 kg.), 31. H₂O, and excess concentrated aqueous NH₃ were evaporated to dryness, the residue treated with 250 cc.

concentrated aqueous NH₃, again evaporated to dryness, the powdered NH₄ salt heated in an

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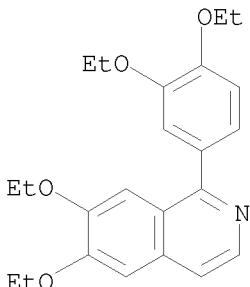
oil bath 3 h. at 160° and 5 h. at 175°, the melt dissolved in boiling H₂O, aqueous NH₃ added, and the whole treated with charcoal and filtered hot to give 162 g. of the amide (XXXII), white crystals, m. 173° (from xylene). The Na derivative of XXXII and PhCH₂Cl gave 100% 3,4-CH₂O₂C₆H₃CH₂CONHCH₂Ph, m. 120°. Eupapaverine or dihydroeupapaverine was catalytically hydrogenated to 1-(3,4-methylenedioxybenzyl)-3-methyl-6,7-methylenedioxy-1,2,3,4-tetrahydroisoquinoline, white crystals, m. 118° (from Et₂O); HCl salt, m. 255°. To 1-norephedrine 2 mols. in 400 cc. ice H₂O was added dropwise 1 mol. PhCH₂COCl, with stirring and addnl. ice cooling, to give PhCH(OH)CHMeNHCOCH₂Ph (XXXIII), m. 133° (from PhMe). XXXIII in tetrahydronaphthalene, with P₂O₅ gave 1-benzyl-3-methoxyisoquinoline, oil; HCl salt, m. 222° (from dilute HCl). Only the phys. consts. of the following compds. are given: 3,4-(MeO)₂C₆H₃CH₂CHMeNHCOCH₂Ph, m. 118° (from alc.); 1-benzyl-3-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline, m. 62° (from Et₂O), [HCl salt (1 H₂O), m. 178° (decomposition)], and the dehydrogenated base, m. 110°; 3,4-CH₂O₂C₆H₃CH₂CHMeNHCH₂Ph, m. 101° (from alc.); 1-benzyl-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline, oil (oxalate, m. 208°; HCl salt, m. 184°), and the dehydrogenated base, m. 116° (HCl salt, m. 265°); R''NHCOCHPhEt, m. 138° (from alc.); 1-(α -ethylbenzyl)-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline, m. 125° (from alc.), and the dehydrogenated base, white plates, m. 143° (HCl salt, white needles, m. 80°); R''NHCOCHPh₂, m. 158° (from 70% alc.); 1-diphenylmethyl-3-methyl-6,7-methylenedioxy-3,4-dihydroisoquinoline, m. 156° (from alc.), and the dehydrogenated base, m. 182° [HCl salt (1 H₂O), m. 121-2° (decomposition)].

IT 719989-88-5P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Synthetic investigations in the isoquinoline series. I)

RN 719989-88-5 HCPLUS

CN Isoquinoline, 1-(3,4-diethoxyphenyl)-6,7-diethoxy- (CA INDEX NAME)



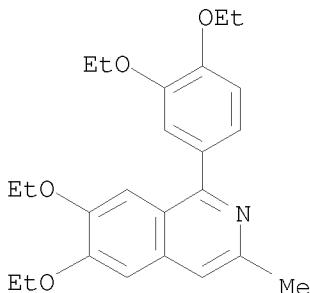
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 283 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1951:32873 HCPLUS
DOCUMENT NUMBER: 45:32873
ORIGINAL REFERENCE NO.: 45:5726a-d
TITLE: Isoquinoline derivatives

STN

INVENTOR(S): Bruckner, Gyozo; Fodor, Gabor; Kiss, Joczef
PATENT ASSIGNEE(S): Servita Gyogyszeryar es Vegyipari R.T.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

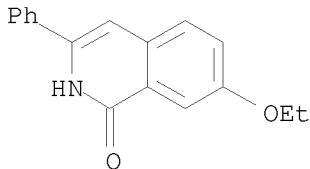
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 645139	-----	19501025	GB 1947-27069	19471008 <--
AB	1-Substituted-3-alkyl-6,7-dialkoxyisoquinolines which have spasm-relieving effects several times those of papaverine and are much less poisonous were prepared from o-dialkoxybenzenes. EtCOCl 45 g. was added in 30 min. at 0° to 71 g. o-(EtO)2C6H4, 60 g. AlCl3, and 250 g. PhNO2, the mixture stirred 2 hrs., hydrolyzed with ice and HCl, and the PhNO2 layer separated, washed, dried, and distilled to give 80% 3,4-(EtO)2C6H3COEt (I), b5 141-5° m. 37°. Me2CHCH2ONO 23.2 g. was added in 1 hr. to a cooled mixture of 37.6 g. of 20% HCl in Et2O, 200 cc. MeOH, and 44.4 g. I, and the mixture neutralized with CaCO3, filtered, concentrated at reduced pressure to give 3,4-(EtO)2C6H3CO(:NOH)Me, m. 121° (from 50% alc.), hydrogenated with Pt oxide catalyst to 3,4-(EtO)2C6H3CH(OH)CH(NH2)Me (II), m. 146-7° (from C6H6). BzCl 4.5 g. added as a 25% solution in C6H6 with stirring to 8 g. II.-HCl in 100 cc. H2O at 40°, with the alkalinity maintained by adding 5 N NaOH, gave 84% 3,4-(EtO)2C6H3CH(OH)CH(NHBz)Me (III), colorless needles, m. 168°. III 7.5 g., 160 cc. PhMe, and 10 cc. POC13 boiled 1 hr. and made alkaline gave 73% 1-phenyl-3-methyl-6,7-diethoxyisoquinoline, m. 125-6° (from dilute MeOH); HCl salt, m. 230°. Other 1-substituted 3-methyl-6,7-diethoxyisoquinolines similarly prepared were as follows: Me, m. 96-7°; 3,4-diethoxyphenyl, m. 96-7° (HCl salt, m. 214-16°); PhCH2, m. 85-6° [HCl salt, m. 213-15° (decomposition)]; 3,4-dimethoxyphenyl, m. 111-12° (HCl salt, m. 221.5°); 3,4-diethoxybenzyl, m. 117-18° (HCl salt, m. 201-2°).			
IT	873404-59-2P, Isoquinoline, 1-(3,4-diethoxyphenyl)-6,7-diethoxy-3-methyl-			
RL: PREP (Preparation)	(preparation of)			
RN	873404-59-2 HCPLUS			
CN	Isoquinoline, 1-(3,4-diethoxyphenyl)-6,7-diethoxy-3-methyl- (CA INDEX NAME)			



L13 ANSWER 284 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1951:24320 HCPLUS
 DOCUMENT NUMBER: 45:24320
 ORIGINAL REFERENCE NO.: 45:4271g-i, 4272a-d
 TITLE: 1-Hydroxyisoquinolines
 INVENTOR(S): Ulliyott, Glenn E.
 PATENT ASSIGNEE(S): Smith, Kline & French Laboratories
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2538341		19510116	US 1949-116867	19490920 <--

GI For diagram(s), see printed CA Issue.
 AB Compds. of the general formula (I) where R' is H, an alkyl not containing more than 10 C atoms, a Ph or phenylalkyl group the alkyl portion of which contains not more than 3 C atoms, R'' and R''' are H, HO, Me, MeO, EtO, H₂N, or AcNH, the said substituents being so chosen that the number of N atoms in the substituents does not exceed 1, are rearranged to give intermediate derivs. of the structure (II) which are then dehydrated to the dihydroisoquinolone (III). Thus, 28 cc. of 40% NaOH added to 79.8 g. aminophthalidylmethane-HCl in 100 cc. warm H₂O, and the solution heated on the steam bath give 68.3 g. crystalline 4-hydroxy-3,4-dihydro-1(2H)-isoquinolone (IV). IV (1 part) added to 3-6 parts concentrated H₂SO₄ kept below 70°, and the whole heated 1-3 hrs. on the steam bath, cooled, and poured into ice H₂O give 1(2H)-isoquinolone (V) (when no m.p. is given here, none was reported). In similar fashion are prepared the following substituted derivs. of V: 3-Me, 3-Et, 3-Pr (VI), 3-Bu (VII), 3-Am (VIII), 3-Ph, 3,6,7-EtMe₂, 3,5,7-MeCl₂, 7-Et, 3,6,7-Pr(MeO)₂, 3,7,8-Bu(MeO)₂, 3,7-Ph(EtO), 3,6,7-PhCH₂(HO)₂ and 7,3-Br(PhCHMeCH₂). 1-Nitro-1-phthalidylpropane, m. 94-6°, in 20 ml. concentrated H₂SO₄ added dropwise with stirring to 11 g. KNO₂ in 33 ml. concentrated H₂SO₄ maintained below 5°, then kept 3 hrs. below 10° and 16 hrs. at room temperature give 1-(6-nitrophthalidyl)-1-nitropropane (IX), m. 95-8° (from alc.). IX (30 g.) in 160 cc. of AcOH is reduced over PtO₂ at 60-80° to 1-(6-aminophthalidyl)-1-nitropropane (X), m. 182-4°. X is reduced over Pd on C in saturated aqueous solution containing 1 equivalent of HCl, under 50 lb. H, the solution filtered, and the filtrate made alkaline with 40% NaOH to rearrange the 1-amino-1-(6-aminophthalidyl)propane to 7-amino-3-ethyl-3,4-dihydro-4-hydroxy-1(2H)-isoquinolone (XI), m. 216-17°. XI (21 g.) in 64 cc. concentrated H₂SO₄ as above gives 3-ethyl-7-amino-1(2H)-isoquinolone, m. 202-3° (from alc.); N-Ac derivative, m. 276-8°; N-butyryl derivative (no m.p. given). X is methylated with HCHO and HCO₂H to 1-(6-dimethylaminophthalidyl)-1-nitropropane which is reduced, rearranged, and dehydrated as above to give 3-ethyl-7-dimethylamino-1(2H)-isoquinolone.
 IT 855623-21-1P, Isocarbostyryl, 7-ethoxy-3-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 855623-21-1 HCPLUS
 CN 1(2H)-Isoquinolinone, 7-ethoxy-3-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L13 ANSWER 285 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1950:30107 HCAPLUS

DOCUMENT NUMBER: 44:30107

ORIGINAL REFERENCE NO.: 44:5859c-i, 5860a

TITLE: Reexamination of the diisohomogenol structure

AUTHOR(S): Doering, W. v. E.; Berson, Jerome A.

CORPORATE SOURCE: Columbia Univ.

SOURCE: Journal of the American Chemical Society (1950), 72, 1118-23

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

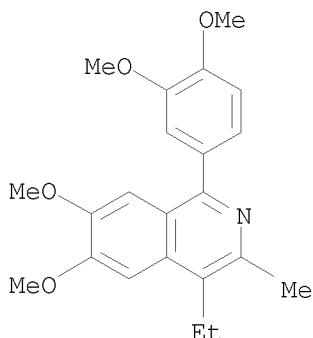
LANGUAGE: Unavailable

AB Diisohomogenol (I) on CrO₃ oxidation gives

3-(2-veratroyl-4,5-dimethoxyphenyl)-2-pentanone (II), m. 156.2-7° (m.ps. corrected); p-nitrophenylhydrazone, light yellow, m. 177.8-8.8°; further reaction (96 hrs.) with p-O₂NC₆H₄NHNH₂ in EtOH containing a little AcOH gives a brick-red powder, m. 190-1°; II was formulated by Muller and Horvath (C.A. 38, 2951.9) as hydroxyketodiisohomogenol. II with MeMgI in PhOMe evolves 0.21-0.36 mol. CH₄, consumes 1.70-1.95 mols. reagent, and thus adds 1.34-1.63 mols.; the reaction product is C₂₄H₃₄O₆, m. 131-4°. II (2 g.) in 20 cc. C₆H₆ and 40 cc. EtOH, saturated at 0° with NH₃ and heated 4.5 hrs. at 70-80°, gives 1.68 g. (crude) 1-(3,4-dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisoquinoline (III), m. 156.9-7.6°, absorption maximum at 249 and 338 mμ (log ε 4.68 and 3.91), inflection at 285 mμ (log ε 3.92); (picrate, canary-yellow, m. 225-7°). II (1 g.) and 1.175 g. NH₂OH.HCl in 4.4 cc. absolute EtOH and 4.4 cc. C₅H₅N, refluxed 3 hrs., give the N-oxide (IV) of III, m. 222.5-3.5°; oxidation of 700 mg. III with BzO₂H in CHCl₃ gives 480 mg. IV. Reduction of 500 mg. IV with Zn and AcOH gives 280 mg. III. II (1 g.), 5 cc. EtSH, and 3 drops concentrated HCl in 40 cc. AcOH, kept 24 hrs. at room temperature and the residue fractionated from MeOH, give 130 mg. unchanged II, 100 mg. 2-methyl-3-(3,4-dimethoxyphenyl)-5,6-dimethoxyindone (V), blood-red, m. 199-201°, and a residue m. 97.8-9.2° (not identified). II is unchanged in AcOH containing a trace of HCl in 106 hrs. 3,4-(MeO)₂C₆H₃COCl (from 1 g. acid and PCl₅ in CS₂) in 10 cc. CS₂, treated 1.5 hrs. with 0.8 g. 3,4-(MeO)₂C₆H₃Pr and 1.15 g. AlCl₃, gives 1.15 g. 6-veratroyl-3,4-dimethoxy-1-propylbenzene (VI), m. 83.5-4.5°. VI (350 mg.) and 200 mg. KMnO₄ in 8 cc. H₂O, refluxed 30 min., give 25 mg. 6-veratroylveratric acid (VII), m. 218-20°; oxidation of II with HNO₃ gives a mixture of 2,3,6,7-tetramethoxyanthraquinone (m. 342-3°) and VII. 1-(3,4-Dimethoxyphenyl)-3-methyl-4-ethyl-6,7-dimethoxyisobenzopyrylium chloride (VIII) (440 mg.) in 25 cc. CHCl₃ and 10 cc. C₆H₆, shaken with 15 cc. 0.4 M BzO₂H in CHCl₃ and kept 5 min. at

4° and 10 min. at room temperature, gives 60 mg.
 6-veratroyl-3,4-dimethoxypropiophenone (IX), m. 151.4-2.7°; if the reaction of VIII and BzO₂H is extended to 2.5 (or 67) hrs., there results 150 mg. V. IX was formulated by M. and H. as 2-methyl-3-hydroxy-3-(3,4-dimethoxyphenyl)-5,6-dimethoxyindanone. VI (0.35 g.), 8 cc. AcOH, 0.5 cc. concentrated H₂SO₄, and 20 cc. Ac₂O treated (25 min.) at 0-10° with 0.212 g. CrO₃, give 30 mg. IX. The sulfate corresponding to VIII (8 g.) in 50 cc. H₂O, treated with 8 cc. 30% H₂O₂ and warmed 1 hr. on the steam bath, gives 3.9 g.
 3-(2-veratroyloxy-4,5-dimethoxyphenyl)-2-pentanone, m. 128.5-9°.
 While a large part of the exptl. basis on which the structure 1-(3,4-dimethoxyphenyl)-2-methyl-3-ethyl-5,6-dimethoxyindan had been assigned to I has been invalidated, the new evidence leads to the same formulation.

IT 1616-49-5, Isoquinoline,
 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl-
 (and derivs.)
 RN 1616-49-5 HCPLUS
 CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-4-ethyl-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
 (2 CITINGS)

L13 ANSWER 286 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1950:10012 HCPLUS
 DOCUMENT NUMBER: 44:10012
 ORIGINAL REFERENCE NO.: 44:1932e-i,1933a-i,1934a-b
 TITLE: Substitution reactions with metallocorganic compounds.
 IV. The Grignardization of methoxyl-containing aromatic nitriles
 AUTHOR(S): Richtzenhain, Hermann; Nippus, Peter
 SOURCE: Chemische Berichte (1949), 82, 408-17
 CODEN: CHBEAM; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 44:10012
 AB cf. C.A. 43, 205b. When 2,3-(MeO)₂C₆H₃CN (I) is treated with RMgX (II) the 2-MeO in I is replaced by R. Since in 1,2,3-(MeO)₃C₆H₃, no MeO group is replaced, a substituent with an unsatd. linkage seems to be required. To test whether other substituents activate an aromatic MeO group, the action

of II on 2,3-R'-(MeO)C₆H₃CN (III) is studied. III (R' = H) and II do not give any new substitution products, indicating that the CN group alone is insufficient to activate the MeO group. 2,3-(MeO)MeC₆H₃CN (IV), b15 117-18°, is prepared from 2,3-(MeO)MeC₆H₄CONH₂, m. 103°, which, in turn, is prepared via the acid chloride, b17 128°. Refluxing 22 g. IV in 200 cc. Et₂O 6 h. with EtMgBr from 27.5 g. EtBr and separating the ketone from the nonketone with Girard reagent give 18.5 g. 2,3-(MeO)MeC₆H₃COEt, b0.3 86°. IV and PhMgBr give 3,2-Me(MeO)C₆H₃C(:NH)Ph, b0.8 135°, which, heated with 157% HCl, gives 2,3-(MeO)MeC₆H₃Bz, b0.15 117°, m. 38° (2,4-dinitrophenylhydrazone, m. 175°). No substituted nitrile is obtained. To study the effect of Cl in III, 3,2-Cl(MeO)C₆H₃CN (V) is prepared 2,3-MeO(O₂N)C₆H₃CO₂Me, m. 52°, prepared from 2,3-HO(O₂N)C₆H₃CO₂H and CH₂N₂, is saponified and the acid chloride, b12 158°, converted into the amide, m. 123°, which with P₂O₅ gives 2,3-MeO(O₂N)C₆H₃CN (VI), m. 104-5°. Reduction of VI with Pd-BaSO₄ gives the 3-NH₂ analog (VII), m. 94-5°. Diazotization of 19 g. VII in 26 cc. concentrated HCl with 7 g. NaNO₂ and addition of 13 g. Cu powder give 7.8 g. V, b15 123-5°, crystals from EtOH, m. 60°. V and EtMgBr give 3,2-Cl(MeO)C₆H₃COEt, b15 135-40° (2,4-dinitrophenylhydrazone, m. 160°), in addition to traces of nonketone. 3,2-I(MeO)C₆H₃CN (VIII) (22 g.), m. 65-6°, prepared like V in 75% yield, and EtMgBr give 9.1 g. 2-MeOC₆H₄CN, b0.4 82°, which is saponified to 2-MeOC₆H₄CO₂H, m. 100°, in addition to 3.1 g. unchanged VIII. 3,4-, 2,5-, and 2,6-(MeO)2C₆H₃CN react normally with II. Refluxing 22.4 g. 2,3,5-(MeO)2(CH:NOH)C₆H₂CH:NOH, m. 187°, with 60 cc. SOC₁₂ in 200 cc. CHCl₃ gives 100% 1,5-di-CN analog (IX), m. 155°. Heating 18.8 g. IX with EtMgBr from 32.7 g. EtBr 5 h. at 70-80° gives 75% 2,3,5-Et(MeO)(EtCO)C₆H₂CN, needles, m. 110° in addition to a ketazine, C₂₆H₃₀O₂N₄, feathered yellow needles, m. 175-7°. Refluxing 66 g. 2,3,5-(MeO)2(Pr)C₆H₂CH:NOH 4 h. with 70 g. NaOAc in 280 cc. Ac₂O gives the CN analog (X), b1.3 138°. Refluxing 25.9 g. X with MeMgI in ether gives 6.6 g. alkali-soluble starting material and 7.8 g. 5,2,3-Pr(MeO)2C₆H₂Ac, yellow oil, b0.5 112° (2,4-dinitrophenylhydrazone, red needles, m. 159-60°). X and EtMgBr give 5,2,3-Pr-(MeO)2C₆H₂COEt, b0.5 121-4°, and a nonketonic fraction with 26.45%, MeO. 2,3,4-(MeO)3C₆H₂CN and EtMgBr give 45% 2,3,4-Et(MeO)2C₆H₂CN, b0.6 105°, and 35% 2,3,4-(MeO)3C₆H₂COEt, b0.2 118-19°. 3,4,5-(MeO)3C₆H₂CN (30 g.) and EtMgBr give 21 g. of a mixture of alkali-insol. ketones which, saponified with 100 cc. concentrated H₂SO₄, gives 7 g. 4,3,5-Et(MeO)2C₆H₂COEt, m. 72° [oxime (XI), m. 94-5°], and 4,3,5-HO(MeO)2C₆H₂COEt. Treating 3 g. XI in 30 cc. ether 2 h. with 3 g. PCl₅, decomposing the mixture with H₂O, and refluxing the reaction product 4 h. with 50 cc. EtOH and 25 cc. HCl give 68% 4,3,5-Et-(MeO)2C₆H₂.HCl; free base (XII), m. 157-8°. Diazotization of XII and demethylation of the product with HBr-AcOH give ethylphloroglucinol. Oxidation of 19.7 g. 5-nitrovanillin in 100 cc. N NaOH with 100 cc. 3% H₂O₂ 20 h. at 20° gives 10.4 g. 3,2,5-MeO(HO)2C₆H₂NO₂, orange leaflets, m. 139°, which, methylated with Me₂SO₄ and 40% KOH at 50° gives 7.4 g. 2,3,5-(MeO)3C₆H₂NO₂ (XIII), yellow needles, m. 77°; from the alkaline solution 2.1 g. 2,3,5-HO(MeO)2C₆H₂NO₂, orange needles, m. 130-1° is isolated. Reduction of XIII with Raney Ni at 40° gives 2,3,5-(MeO)3C₆H₂NH₂, pale yellow oil, b0.4 119°. Heating 32.2 g. 2,3-(MeO)2C₆H₃CHO and 20 g. PhNH₂ 3 h. in 50 cc. EtOH gives 2,3-(MeO)2C₆H₃CH:NPh (XIV), pale yellow

prisms, m. 90°. Keeping 24.1 g. XIV with EtMgBr from 13 g. EtBr in 100 cc. ether overnight, refluxing the mixture 2 h., and decomposing it with NH₄Cl give 24.6 g. 2,3-(MeO)C₆H₃CHEtNHPH, m. 105°. Condensation of 19.5 g. 3,4-(MeO)C₆H₃CH(OMe)CH₂NH₂ in 75 cc. C₅H₅N with 22 g. 2,3-(MeO)C₆H₃COCl gives 34 g. 3,4-(MeO)C₆H₃CH(OMe)CH₂NHCOC₆H₃(OMe)₂(2,3), m. 119°, which (5 g.), refluxed 1 h. with 10 g. POC₁₃ in 50 cc. xylene, gives 28% 6,7-dimethoxy-1-(2,3-dimethoxyphenyl)isoquinoline, prisms, m. 134-5°. Refluxing 36 g. 2,3-(MeO)C₆H₃CH:CHMe (XV) in 110 cc. Et₂O with EtMgBr 8 h. gives 0.6 g. o-isoeugenol, m. 74.6°, whereas the main part of XV is recovered unchanged. Heating 80 g. 2,3-(MeO)C₆H₃CH:C(CN)CO₂H in 160 g. quinoline with some Cu bronze 4 h., extracting the acidified mixture with ether, washing the ether extract with dilute

NaOH, and distilling the residue of the dried ether extract give 34 g. 2,3-(MeO)C₆H₃CH:CHCN, b₁.5 145-7°, m. 77°, which, with EtMgBr gives a compound, C₂₄H₂₈O₄N₂, m. 186-7° in small yield. Refluxing 16.2 g. 2,3-(MeO)C₆H₃Bz (XVI) with PhMgBr 4 h. in ether gives 13.4 g. [2,3-(MeO)C₆H₃]Ph₂COH (XVII), prisms, m. 106°. 2,3-(MeO)C₆H₃CO₂Et and PhMgBr refluxed 4 h. in 100 cc. ether give 14.9 g. XVII in addition to a small amount of Ph₂ and XVI. Treating 1,2-MeOC₁₀H₆COCl, b₀.3 110-15°, with concentrated NH₄OH gives the amide, needles from EtOH, m. 158°, which, heated with PCl₅, gives the 2-nitrile (XVIII), needles, m. 42-3°. Refluxing 11 g. XVIII with EtMgBr in ether gives 0.6 g. nonketonic product, b₀.3 200°, from which no uniform compound is isolated. The ketonic fraction is 1,2-MeOC₁₀H₆COEt, b₀.3 125-6°, m. 50-1°. Refluxing 18.3 g. XVIII with PhMgBr in ether 5 h. gives 7 g. 1,2-MeOC₁₀H₆Bz, b₀.6 170-82° m. 71-2°. 4,3,2-C₁(MeO)C₁₀H₅CO₂H, m. 189°, is converted via the amide, m. 178-9° with PCl₅ into 90% 2-nitrile analog, m. 146-7°, which is not changed after boiling 5 h. with EtMgBr in ether. 2,3,4-Br(MeO)C₁₀H₅CN, m. 150-1°, prepared from the 2-CONH₂ analog, m. 181-2° with PCl₅, is not changed after being boiled 5 h. with EtMgBr. When 32.6 g. 2,3-(MeO)C₆H₃CN is treated 0.5 h. with EtMgBr from 44 g. EtBr, the mixture refluxed 6 h. with 50 g. AcCl, and the solution decanted from the precipitate; 8 g. 2,3-Et(MeO)C₆H₃CN (XIX) is isolated

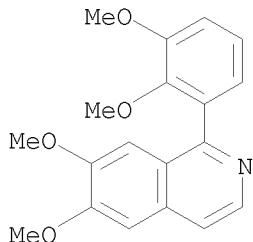
from the solution. Decomposing the precipitate gives 12 g. XIX in addition to 4.5 g. of a fraction, b₀.3 135-45° from which 3.3 g. crystals, m. 70-80°, are obtained; they are sepal, with petr. ether into the 2 stereoisomeric 2,3-Et(MeO)C₆H₃CET:NAc, m. 92-3° and 119-21°.

IT 500998-16-3P, Isoquinoline,
1-(2,3-dimethoxyphenyl)-6,7-dimethoxy-
RL: PREP (Preparation)

(preparation of)

RN 500998-16-3 HCPLUS

CN Isoquinoline, 1-(2,3-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L13 ANSWER 287 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1950:7606 HCAPLUS
DOCUMENT NUMBER: 44:7606
ORIGINAL REFERENCE NO.: 44:1510f-i,1511a-c
TITLE: Attempts to find new spasmolytics. VIII. The synthesis of 6,7-diethoxy-3-alkyl- and 6,7-diethyl-3-phenyl-isoquinolines
AUTHOR(S): Fodor, Gabor; Kiss, Jozsef; Szekerke, Maria
SOURCE: Journal of the Chemical Society (1949)
1681-2
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 44:7606
AB cf. C.A. 43, 1423b. o-C₆H₄(OEt)₂ (33.4 g.), 21.2 g. PrCOCl, and 28 g. AlCl₃ in 130 PhNO₂ give 73% 3,4-diethoxybutyrophenone, (I), b5 170-5°, m. 49-9.5°; 3,4-diethoxyvalerophenone (II), b4 170-3°, m. 45-6°, 87%; 3,4-diethoxy-a-phenylacetophenone (III), b4-5 206-15°, m. 90-1°, 74%. I (11.8 g.) in 60 ml. C₆H₆, treated with 10 g. 20% ether-HCl and then with 6 g. iso-BuONO, gives 87% of the α-oximino derivative (IV), m. 102-3°; that (V) of II, yellow, m. 95-6°, 75%; that (VI) of III, yellow, m. 146°, 77%. IV (10.7 g.) in 350 ml. EtOH and 8 g. EtOH-HCl, reduced over 6 g. Pd-C and then in 160 ml. 50% EtOH over 0.7 g. Pt oxide, gives (after 24 hrs.) 47% 2-amino-1-(3,4-diethoxyphenyl)-1-butanol (VII), whose HCl salt m. 181-2°; the N-Bz derivative of VII m. 158-9° (97%); N-(3,4-dimethoxybenzoyl) derivative, m. 154-5°, 90%; 1 g. VII in 18 ml. H₂O and 0.7 g. PhCH₂COCl in 7 ml. C₆H₆ give 97% of the N-(phenylacetyl) derivative, m. 143-5°. V (17 g.) in 200 ml. EtOH and 30 ml. 5 N EtOH-HCl, reduced over 5 g. Pd-C and then in 260 ml. 60% EtOH over 1 g. Pt oxide, gives 20% 2-amino-1-(3,4-diethoxyphenyl)-1-pentanol, whose HCl salt, with 1 mol. AcOEt, m. 192-3°; Bz derivative, m. 162-3°; O,N-bis(phenylacetyl) derivative, m. 140-1°, 71%; N-(3,4-dimethoxybenzoyl) derivative, m. 154-5°, 90%. VI, reduced in 200 ml. EtOH and 8 ml. 5 N EtOH-HCl with Pd-C and then in 135 ml. 80% EtOH over 0.7 g. Pt oxide, gives 59% 2-amino-2-phenyl-1-(3,4-diethoxyphenyl)ethanol, m. 142-3°; HCl salt, m. 186-7°; N-Bz derivative, m. 214-15°, 85%; N-Ac derivative, m. 171-2°, 90%. The following were prepared by boiling 1 hr. the acylamide in PhMe with an excess of POCl₃ and crystallizing from 50% EtOH.
6,7-Diethoxy-1-phenyl-3-ethylisoquinoline, m. 100-1°, 75.5% (authors give 3-methyl instead of 3-ethyl); 1-benzyl analog, m.

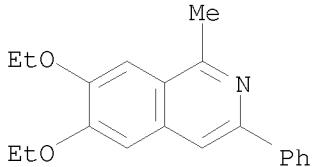
88-9°, 44%; 1-(3,4-dimethoxyphenyl) analog, with 1 mol. H₂O, m.
 98-9°, 66%. 6,7-Diethoxy-1-phenyl-3-propylisoquinoline, m.
 94-5°, 52%; 1-benzyl analog, m. 107-8°, 48%;
 1-(3,4-dimethoxyphenyl) analog, m. 90-1°, 48.5%.
 6,7-Diethoxy-1,3-diphenylisoquinoline, m. 173-4°, 44%;
 6,7-diethoxy-3-phenyl-1-methylisoquinoline, m. 137-8°, 50%. Except
 for the 1,3-di-Ph compound, all exert similar spasmolytic activity and are
 more active than papaverine, but none is an appreciable improvement on the
 1-phenyl-3-methyl compound

IT 855648-10-1P, Isoquinoline, 6,7-diethoxy-1-methyl-3-phenyl-

RL: PREP (Preparation)
 (preparation of)

RN 855648-10-1 HCPLUS

CN Isoquinoline, 6,7-diethoxy-1-methyl-3-phenyl- (CA INDEX NAME)



L13 ANSWER 288 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1950:5538 HCPLUS

DOCUMENT NUMBER: 44:5538

ORIGINAL REFERENCE NO.: 44:1113b-f

TITLE: Synthetic and degradative studies in the isoquinoline series. IV

AUTHOR(S): Fodor, G.; Bruckner, V.; Kiss, J.; Kovacs, J.

SOURCE: Journal of the American Chemical Society (1949), 71, 3694-7

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 42, 8800d. 2,3,4-HO(MeO)2C6H2CO2Me (10 g.) and 6 ml. PhCH₂Cl in 50 ml. absolute EtOH containing 1.1 g. Na give 2-benzyloxy-3,4-dimethoxybenzoic acid (I), m. 95-6°. The acid chloride from 11.5 g. I and 27 g. MeCH(NH₂)CH[C₆H₃(OMe)2]OH (II) give 18 g.

3,4-(MeO)2C₆H₃CH(OH)CH(Me)NHCO₆H₂(OMe)2OH-3,4,2 (III), m. 87-8°; CH₂N₂ in ether gives 1-(3,4-dimethoxyphenyl)-2-(2,3,4-trimethoxybenzamido)-1-propanol (IV), m. 107-8°. 2,3,4-(MeO)3C₆H₂COCl (1.06 g.) and 2.2 g. II also give IV. III (18 g.) in 500 ml. absolute EtOH, treated with 1.05 g. Na in 50 ml. absolute EtOH and 8 ml. PhCH₂Cl, refluxed 8 hrs., and the residue in 500 ml. hot PhMe treated with 25 ml. POCl₃, gives 8 g. of the benzyl ether (IV), m. 147-8°, of

1-(2-hydroxy-3,4-dimethoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline (V), m. 168-9° (95.6% from 6.5 g. IV and 2.5 g. 7% Pd-C in 280 ml. EtOH); picrate, yellow, m. 238-9°; the Me ether of IV m.

105-7°. V is not the compound obtained by Pfeiffer, et al. (C.A. 34, 2383.3), from tetramethylhematoxylonol oxime. Oxidation of 3.7 g. V in 525 ml. hot 0.03% aqueous NaOH with 23.7 g. KMnO₄ in 475 ml. hot H₂O gives 200 mg. 3,4,1,2-(MeO)2C₆H₂(CO₂H)₂, m. 175-7°. III (21.1 g.) and 6.8 g. EtO₂CCOCl in 100 ml. CHCl₃, kept overnight, give 6.5 g.

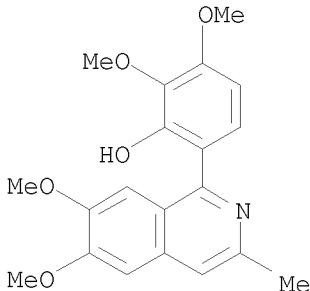
1-(3,4-dimethoxyphenyl)-2-(ethoxyallylamino)-1-propanol (VI), m. 92-3°; the 2-(trichloroacetamido) analog m. 115-16° (0.8 g. from 2.11 g. III). VI (0.94 g.) and 0.8 ml. POC13 in 15 ml. PhMe, refluxed 1 hr. and the residue from the ether extract (183 mg.) boiled 90 min. with 4 ml. 10% NaOH and 5 ml. MeOH, give 57 mg. 3-methyl-6,7-dimethoxy-1-isoquinolinecarboxylic acid (VII), with 1 mol. H₂O, yellow, m. 203-4° (decomposition); 4.5 g. III in 80 ml. HCO₂H, refluxed 48 hrs. and the residue treated with POCl₃ in 100 ml. PhMe, gives 1.2 g. 3-methyl-6,7-dimethoxyisoquinoline (VIII), m. 135-6° [HCl salt, m. 237-8°; picrate (IX), yellow, m. 269-70°; IX results also on the attempted preparation of the picrate of VII]; on heating VII at 200°/1. mm. VIII is formed. The Me ester of VII (from CH₂N₂ in MeOH) m. 151-3° (picrate, m. 216°); Et ester, yellow, m. 86-7° (picrate, golden yellow, m. 176-7°). VII with KMnO₄ gives 3,4,1,2-(MeO)₂C₆H₂(CO₂H)₂.

IT 850858-43-4, Phenol, 6-(6,7-dimethoxy-3-methyl-1-isoquinolyl)-2,3-dimethoxy-

RL: PREP (Preparation)
(and derivs.)

RN 850858-43-4 HCPLUS

CN Phenol, 6-(6,7-dimethoxy-3-methyl-1-isoquinolyl)-2,3-dimethoxy- (CA INDEX NAME)



L13 ANSWER 289 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1950:5537 HCPLUS

DOCUMENT NUMBER: 44:5537

ORIGINAL REFERENCE NO.: 44:1112f-i,1113a-b

TITLE: Esters of papaverine and norpapaverine acids with diethylaminoethanol

AUTHOR(S): Redel, J.; Bouteville, A.

SOURCE: Bulletin de la Societe Chimique de France (1949) 443-6

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Heating 23 g. N-homoveratroylglycine, m. 149-50°, prepared from homoveratroyl chloride and glycine by the Schotten-Baumann reaction, with 15 g. verataldehyde, 7.4 g. fused AcONa, and 27.5 g. Ac₂O, followed by EtOH addition, gives 7.7 g. (22%) α -homoveratroylamino-3,4-dimethoxycinnamic acid azlactone (I), m. 163-4°. The α -veratroylamino analog (II), m. 193-4°, is prepared similarly in 73% yield from N-veratroylglycine, m. 189-90°. Heating 7.5 g. I

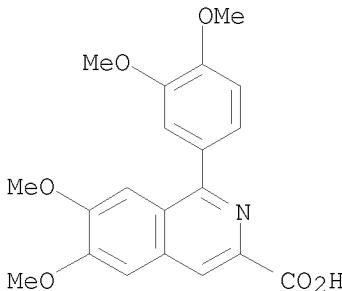
in 75 cc. MeOH with 1.25 Na₂CO₃, followed by addition of petr. ether, gives 7 g. Me α -homoveratroylamino-3,4-dimethoxycinnamate (III), m. 126-7°. Hydrogenation of III gives (3,4-dimethoxyphenyl)-N-homoveratroyl- β -alanine Me ester (IV), m. 89-92°. Refluxing 9.6 g. IV in C₆H₆ with 9.6 g. POCl₃ gives 7.5 g. Me dihydropapaverine-3-carboxylate (V), m. 125-8° (cf. C.A. 28, 1703.3). Dehydrogenation of V with S at 155° gives Me papaverine-3-carboxylate, m. 178° (C.A. 33, 5004.5), which on hydrolysis with 2% alc. NaOH gives 3-carboxypapaverine (VI), m. 175-6°. 2-Diethylaminoethyl papaverine-3-carboxylate-HCl (VII), m. 113-14°, prepared from VI and Et₂NCH₂CH₂Cl (VIII) in iso-PrOH, and 2-diethylaminoethyl norpapaverine-3-carboxylate-HCl (IX), m. 191-2°, prepared from VIII and 3-carboxynorpapaverine (X), m. 212-13°, were evaluated as spasmolytical compds. on the rabbit intestine contracted with acetylcholine (IX more active than VII) or with BaCl₂ (VII more active than IX). Me α -veratroylamino-3,4-dimethoxycinnamate, m. 150-1°, prepared from II by alcoholysis, is hydrogenated to 3,4-dimethoxy-N-veratroyl- β -alanine Me ester, m. 148°, which on cyclization gives Me dihydronorpapaverine-3-carboxylate, m. 144-5°. Heating with S yields Me norpapaverine-3-carboxylate, m. 210-13°, which was saponified to X.

IT 855692-05-6, 3-Isoquinolinecarboxylic acid,
1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-

(and esters)

RN 855692-05-6 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L13 ANSWER 290 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1949:6485 HCPLUS
DOCUMENT NUMBER: 43:6485
ORIGINAL REFERENCE NO.: 43:1423a-i,1424a-b
TITLE: Synthesis of 6,7-diethoxy-3-methylisoquinolines
AUTHOR(S): Bruckner, G., Jr.; Fodor, G.; Kiss, J.; Kovacs, J.
SOURCE: Journal of the Chemical Society (1948)
885-90
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 43:6485

AB The preparation is described of 1-substituted
 6,7-diethoxy-3-methylisoquinolines by 2 alternative routes.
 3,4-(EtO)₂C₆H₃CH:CHMe (preparation in 85% yield given) yields 85% of the
 ψ -nitrosoite (I), C₁₃H₁₈O₅N₂, m. 124.5-5.5° (decomposition). I (80
 g.) in 240 cc. Ac₂O, treated dropwise with ice cooling with Ac₂O containing 4
 drops H₂SO₄, gives 59% 2-nitro-1-(3,4-diethoxyphenyl)propyl acetate (II),
 m. 75°. II (30 g.) in 170 cc. EtOH, 80 cc. AcOH, and 26 cc. concentrated
 HCl, reduced in a Hg electrode apparatus (20% H₂SO₄ as anolyte) with a c.d. of
 0.07 amp./sq. cm. at a temperature not above 60°, gives 65.8%
 ψ -2-acetamido-1-(3,4-diethoxyphenyl)propanol (III), m. 128-31°;
 3 g. III in 10 cc. MeOH and 1.26 cc. 32.1% MeOH-HCl, evaporated to dryness in
 a desiccator over CaCl₂ and KOH, gives
 ψ -2-amino-1-(3,4-diethoxyphenyl)propyl acetate-HCl, m. 162°;
 the free base has the same m.p. as III. A solution of 3.6 g. III in 38 cc.
 10% H₂SO₄ (prepared by heating on the steam bath), cooled and basified with
 10% NaOH, gives ψ -2-amino-1-(3,4-diethoxyphenyl)propanol (IV), m.
 116-17° (HCl salt, m. 176-7°). For the preparation of the
 following acyl derivs., it is not necessary to isolate IV, since the
 neutral solution can be treated with a 25% C₆H₆ solution of the acid chloride
 and the equivalent quantity of NaOH, with stirring for 1 h.: Bz, m.
 129°, 81%; veratroyl, m. 149-51°, 87%;
 3,4-diethoxybenzamido, m. 158.5°, 81.8%;
 3,4-diethoxyphenylacetamido, m. 98-9°, 41%; phenylacetamido, m.
 132°, 60%. o-C₆H₄(OEt)₂ (174 g.), added to 147 g. AlCl₃ in
 650 g. PhNO₂, the mixture cooled to -5°, treated (30 min.) with 110
 g. EtCOCl, and kept 2 h. at 0° to -5°, gives 73.1%
 3,4-diethoxypropiophenone (V), pale yellow, b₃₂ 181-4°, m.
 38-9°; 3,4-(HO)C₆H₃COEt (41.5 g.) and 60 g. EtBr in 200 cc. EtOH,
 treated dropwise with 80 cc. 25% EtOH-KOH, the mixture refluxed 3 h., 10 g.
 EtBr added, and refluxed an addnl. 6 h., give 54% V and 18.5 g. mono-Et
 derivative V (44.4 g.) in 200 cc. anhydrous MeOH and 37.6 g. 20% ether-HCl,
 treated dropwise (30-45 min.) with 23.7 g. iso-BuNO₂, the mixture kept 12 h.
 at room temperature, neutralized with CaCO₃, and evaporated in vacuo, gives
 90% of
 the α -isonitroso derivative (VI), pale yellow, m. 121°; if the
 reaction is carried out in C₆H₆, VI crystallizes from the reaction mixture
 VI (16.5 g.) in 200 cc. EtOH, added to 2 g. Pt oxide in 50 cc. EtOH saturated
 with H, the product treated with 49.5 cc. 4 N EtOH-HCl, and shaken with H
 8 h. at room temperature, gives the α -NH₂ derivative of V, whose HCl salt m.
 203°; most of the base was further hydrogenated (after
 neutralization of the excess HCl) 4 h., giving 18 g. of the HCl salt
 (VII), m. 199°, of 2-amino-1-(3,4-diethoxyphenyl)propanol (VIII),
 m. 146-7°. VIII (3.8 g.) in 60 cc. C₅H₅N and 1.6 g. Ac₂O, allowed
 to stand 24 h., gives 78.3% of the N-Ac derivative, m. 124-5°; VII and
 Ac₂O in C₅H₅N give 64% of the O,N-di-Ac derivative, m. 134-5°; 8 g. VII
 and 5.4 g. BzCl give 84% of the N-Bz derivative, m. 168°; veratroyl
 derivative, m. 110°, 79.4%; diethoxybenzamido compound, m. 124°,
 69.7%; 3,4-diethylphenylacetamido compound, m. 112-13°, 58.4%;
 phenylacetamido compound, m. 135°, 75.4%. The acyl derivs. of IV in
 CHCl₃ or PhMe and POCl₃, refluxed 40-120 min., give the following
 isoquinolines: 6,7-diethoxy-1,3-dimethyl, m. 96-7°, 74%; the isomer
 from VII yields 92.3% of the same base; 6,7-diethoxy-1-phenyl-3-Me, m.
 125-6° (HCl salt, m. 230°);
 6,7-diethoxy-1-(3,4-dimethoxyphenyl)-3-Me, m. 111-12° (HCl salt, m.
 236.5-7°), 80 and 65% from the 2 isomers;

6,7-diethoxy-1-(3,4-diethoxyphenyl)-3-Me, m. 96-7° (HCl salt, m. 222°), 50 and 63% from the 2 isomers; 6,7-diethoxy-1-benzyl-3-Me, m. 86° [HCl salt, m. 213-15° (decomposition)]; 6,7-diethoxy-1-(3,4-diethoxybenzyl)-3-Me, m. 117-18° (HCl salt, m. 201-2°); 3,4-(EtO)₂C₆H₃COCHMeNH₂ forms 80% of a Bz derivative, m. 124.5°; refluxed 4 h. with POCl₃ in PhMe, this yields 2-phenyl-5-(3,4-diethoxyphenyl)-4-methyloxazole, pale yellow, m. 114-14.5° (HCl salt, m. 166-7°); the free base in aqueous EtOH shows a bluish violet fluorescence. The isoquinolines (except the 1-Me derivative) have a higher spasmolytic activity and a lower toxicity than papaverine. The 1-Ph derivative has the same activity as tetraethylpapaveroline and as the alkoxyphenyl and the alkoxybenzyl derivs. of 6,7-diethoxy-3-methylisoquinoline; it is not toxic and can be used medicinally.

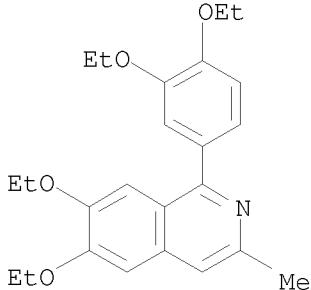
IT 873404-59-2P, Isoquinoline,
1-(3,4-diethoxyphenyl)-6,7-diethoxy-3-methyl-

RL: PREP (Preparation)

(preparation of)

RN 873404-59-2 HCPLUS

CN Isoquinoline, 1-(3,4-diethoxyphenyl)-6,7-diethoxy-3-methyl- (CA INDEX NAME)



L13 ANSWER 291 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1948:41810 HCPLUS

DOCUMENT NUMBER: 42:41810

ORIGINAL REFERENCE NO.: 42:8800c-g

TITLE: Synthetic and degradative studies in the isoquinoline series. III

AUTHOR(S): Bruckner, V.; Fodor, G.; Kovacs, J.; Kiss, J.

CORPORATE SOURCE: Univ. Szeged, Hung.

SOURCE: Journal of the American Chemical Society (1948), 70, 2697-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 40, 6481.3. Pfeiffer, et al. (C.A. 34, 2383.3), obtained a compound from brazilin for which they suggested the structure 1-(2-hydroxy-4-methoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline (I); attempted synthesis of I led to a compound to which they assigned the structure of the 7,8-di-MeO isomer (II). 2,4-HO(MeO)C₆H₃CO₂Me (18 g.) and 13 ml. PhCH₂Cl in 100 ml. EtOH containing 2.3 g. Na, refluxed 12 hrs. and the product saponified with 6 g. KOH in 20 ml. H₂O, give 9.5 g.

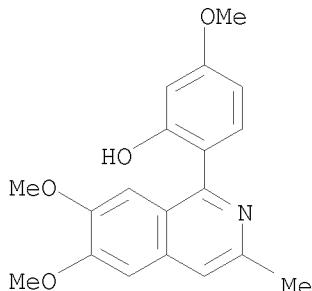
2-(benzyloxy)-4-methoxybenzoic acid (III), m. 103°. III (9.5 g.) in 20 ml. PhMe, heated at 35-40° with 16 ml. SOC12 until HCl is evolved, the SOC12 removed in vacuo, the residue in 50 ml. hot absolute PhMe added dropwise to 21.3 g. 3,4-(MeO)2C6H3CH(OH)CHMeNH2 in 500 ml. boiling PhMe and the mixture refluxed 15 min., gives 91% 1-(3,4-dimethoxyphenyl)-2-[2-(benzyloxy)-4-methoxybenzamido]-1-propanol (IV), m. 139-40°. IV (14.5 g.) in 300 ml. hot PhMe, treated with 15 ml. POC13 and refluxed 1 hr., gives 75% 1-[2-(benzyloxy)-4-methoxyphenyl]-3-methyl-6,7-dimethoxyisoquinoline (V), m. 83-4° (HCl salt, yellowish green, m. 221-2°). V (15 g.) in 300 ml. absolute EtOH, reduced over Pd-C, gives 96% I, m. 143-4° [HCl salt, yellow, m. 271°; picrate, yellow, m. 274-6° (decomposition), as reported by P., et al.; Me ether, m. 144°]. Oxidation of I with alkaline KMnO4 gives 4,5,1,2-(MeO)2C6H2(CO2H)2. Thus, the synthetic product of P., et al., is I and not II and the structure of the product from brazilin is still undetd.

IT 850858-42-3P, Phenol, 2-(6,7-dimethoxy-3-methyl-1-isoquinolyl)-5-methoxy-

RL: PREP (Preparation)
(preparation of)

RN 850858-42-3 HCPLUS

CN Phenol, 2-(6,7-dimethoxy-3-methyl-1-isoquinolyl)-5-methoxy- (CA INDEX NAME)



L13 ANSWER 292 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1948:775 HCPLUS

DOCUMENT NUMBER: 42:775

ORIGINAL REFERENCE NO.: 42:173a-h

TITLE: Availability of safrole for the synthesis of 1-substituted 3-methyl-6,7-diethoxyquinolines

AUTHOR(S): Kovacs, Jozsef

CORPORATE SOURCE: Univ. Szeged, Hung.

SOURCE: Acta Univ. Szegediensis, Acta Chem. et Phys. [N.S.] (1943), 1, 109-44

DOCUMENT TYPE: Journal

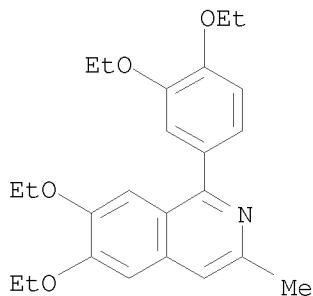
LANGUAGE: Unavailable

AB A cheap method for the production of 3,4-diethoxy-1-propenylbenzene using safrole (I) as the basic substance was sought. The best procedure found was treating I under pressure with KOH in EtOH or MeOH, thus obtaining a mixture of methoxyisoeugenol and methoxyisochavibetol. This mixture in absolute alc. was treated with small amts of concentrated H2SO4 and

4-propenylpyrocatechol added, and, in the presence of K₂CO₃ and EtI or EtBr, ethylated to 3,4-diethoxy-1-propenylbenzene (II), m. 54°, in 85% yield. The following were also obtained:
 3,4-diethoxy-1-propenylbenzene pseudonitrosite (III), m. 124.5-5.5° (decomposition), 53% yield calcd on the amount of the II used;
 1-(3,4-diethoxyphenyl)-2-nitropropyl acetate (IV), colorless large prisms, m. 75°, prepared in 59% yield from III;
 3,4-diethoxy-1-(2-nitropropenyl)benzene, prepared from IV, large prisms or fine needles or shiny thin sheets according to the alc. content of solvent, m. 59.5°; 1-(3,4-diethoxyphenyl)-2-acetamido-1-propanol (V), prepared from IV in 65.8% yield, white crystals, m. 128°;
 1-(3,4-diethoxyphenyl)-2-aminopropyl acetate-HCl, from V, m. 162°;
 1-(3,4-diethoxyphenyl)-2-(N-acetylhydroxamino)-1-propanol (VI), from IV in 80% yield, m. 146.5° (its alc. solution gives a violet color with FeCl₃ solution); 1-(3,4-diethoxyphenyl)-2-hydroxaminopropyl acetate-HCl, prepared from VI, m. 138.5-9.5° (decomposition);
 1-(3,4-diethoxyphenyl)-2-amino-1-propanol, prepared from V in 52% yield, m. 116-20° (HCl salt m. 176-7°);
 1,3-dimethyl-6,7-diethoxyisoquinoline, prepared from V in 74% yield, m. 96-7°; 1-(3,4-diethoxyphenyl)-2-benzamido-1-propanol (VII), 81% from V, m. 128.5-9°. 1-Phenyl-3-methyl-6,7-diethoxyisoquinoline (prepared from VII with POCl₃ to obtain the crystalline hydrochloride, m. 230° (decomposition), which was filtered off and alkalinized), fine needles, m. 125-6° (82% combined yield of free base plus HCl salt).
 1-(3,4-Diethoxyphenyl)-2-(3,4-diethoxybenzamido)-1-propanol (VIII), prepared from V in 81.8% yield, fine needles, m. 158.5°.
 1-(3,4-Diethoxyphenyl)-3-methyl-6,7-diethoxyisoquinoline-HCl, 50% from VIII, yellowish green prisms, m. 214-16°; free base m. 96-7°. 1-(3,4-Diethoxyphenyl)-2-phenylacetamidopropyl phenylacetate (IX), prepared from V in 60% yield, fine needles, m. 132°. 1-Benzyl-3-methyl-6,7-diethoxyisoquinoline-HCl (obtained from IX), long needles, m. 213-15° (decomposition); alkali yields the free base, colorless octahedrons, m. 85-6°.
 1-(3,4-Diethoxyphenyl)-2-veratroylamino-1-propanol, 87% from V, white crystals, m. 149-51°. 1-(3,4-Dimethoxyphenyl)-3-methyl-6,7-diethoxyisoquinoline-HCl (X) m. 221.5°; free base m. 111-12°. 1-(3,4-Diethoxyphenyl)-2-(3,4-diethoxyphenylacetamido)-1-propanol, 41% from X, m. 98-9°.
 1-(3,4-Diethoxybenzyl)-3-methyl-6,7-diethoxyisoquinoline, fine needles, m. 117-18°; HCl salt m. 201-2°. 3,4-Diethoxyphenylacetic acid (XI), prepared by distilling its ester under a vacuum, hexagonal crystals, m. 82°. 3,4-Diethoxy- α -toluyl chloride was a yellow oil.

3,4-Diethoxybenzoyl chloride, a white crystalline mass, was prepared in 94.7% yield by treating XI with SOCl₂.

IT 873404-59-2P, Isoquinoline,
 1-(3,4-diethoxyphenyl)-6,7-diethoxy-3-methyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 873404-59-2 HCPLUS
 CN Isoquinoline, 1-(3,4-diethoxyphenyl)-6,7-diethoxy-3-methyl- (CA INDEX NAME)



L13 ANSWER 293 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1948:774 HCPLUS

DOCUMENT NUMBER: 42:774

ORIGINAL REFERENCE NO.: 42:172h-i,173a

TITLE: Derivatives of 3-methyl-7-methoxyisoquinoline

AUTHOR(S): Bruckner, Gyozo, Jr.; Bodnar, Laszlo

CORPORATE SOURCE: Hungarian Biol. Research Inst., Tihany, Hung.

SOURCE: Magyar Biol. Kutatointezet Munkai (1943),

15, 404-10

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB From isosafrole and methylisoeugenol was prepared a series of 3-methylisoquinolines, the structure of which seems to approach that of papaverine, with excellent spasmolytic effects. The following 2-substituted 1-(4-methoxyphenyl)-1-propanols were prepared: benzamido, colorless microcrystals, m. 146°; anisoylamino, m. 153°; veratroylamino, m. 168°; p-ethoxybenzamido, m. 167°; (3,4-methylenedioxybenzamido), prisms, m. 159°; (3,4-methylenedioxyphenylacetamido), m. 141°; cinnamoylamino, prisms, m. 141°. 1-Substituted3-methyl-7-methoxyisoquinolines: Ph, needles, m. 145°; (4-methoxyphenyl), needles, m. 152°; (3,4-dimethoxyphenyl), needles, m. 145°; p-phenetyl, m. 165°; (3,4-methylenedioxyphenyl), microneedles, m. 136°; (3,4-methylenedioxybenzyl), microneedles, m. 149°; styryl, needles, m. 154°. The results proved the existence of a relationship between chemical composition and spasmolytic effect.

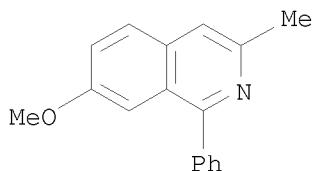
IT 78451-54-4P, Isoquinoline, 7-methoxy-3-methyl-1-phenyl-

RL: PREP (Preparation)

(preparation of)

RN 78451-54-4 HCPLUS

CN Isoquinoline, 7-methoxy-3-methyl-1-phenyl- (CA INDEX NAME)



L13 ANSWER 294 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1947:2285 HCPLUS
 DOCUMENT NUMBER: 41:2285
 ORIGINAL REFERENCE NO.: 41:456i,457a-i,458a-c
 TITLE: Synthesis of 3-methylisoquinolines. II
 AUTHOR(S): Clemo, G. R.; Turnbull, J. H.
 CORPORATE SOURCE: Univ. of Durham, Newcastle-upon-Tyne, UK
 SOURCE: Journal of the Chemical Society (1946) 701-5
 CODEN: JCSOA9; ISSN: 0368-1769
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

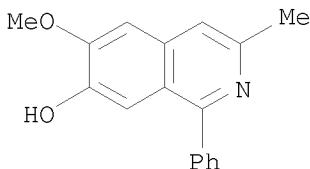
AB cf. C.A. 40, 577.3. $4,3\text{-HO}(\text{MeO})\text{C}_6\text{H}_3\text{CH}_2\text{CHMeNH}_2$ (I) (0.48 g.) in 2 cc. 50% HCO_2H , evapd to dryness in vacuo, gives 0.4 g. of the formate, pinkish white, m. 152-4°, which is readily hydrolyzed by dilute K_2CO_3 ; heated at 145° for 4 hrs., it yields $\text{N-[2-(4-hydroxy-3-methoxyphenyl)isopropyl]formamide}$ (II), m. 96-8°; the aqueous solution gives a blue color with FeCl_3 ; acetylation gives a gummy product of doubtful purity, which could not be cyclized satisfactorily. II (0.45 g.) and 0.37 g. BzCl in 6 cc. xylene, refluxed 2 hrs., give 0.2 g. $\text{N-[2-(4-hydroxy-3-methoxyphenyl)isopropyl]benzamide}$ (III), m. 136-7°. II (0.7 g.) in 35 cc. ice-cold 0.5 N NaOH, treated with 0.6 g. BzCl in 6 cc. ether during 40 min., gives 0.3 g. $\text{N-[2-(4-benzoxy-3-methoxyphenyl)isopropyl]formamide}$ (IV), m. 98-9°; 0.4 g. of IV and 0.8 cc. POCl_3 in 4 cc. CHCl_3 , refluxed 1 hr., give 80 mg. of 7-benzoxy-6-methoxy-3-methyl-3,4-dihydroisoquinoline (V), m. 125-6° (picrate, pale yellow, m. 202-3°); heated with 2 cc. 10% NaOH on the water bath for 1 hr., 90 mg. of the HCl salt of V in 1 cc. EtOH gives 40 mg. 7-hydroxy-6-methoxy-3-methyl-3,4-dihydroisoquinoline (VI), m. 141-3°. I (0.5 g.) in 40 cc. 0.5 N NaOH, treated dropwise with 0.94 g. BzCl in 3 cc. C_6H_6 , gives 0.5 g. $\text{N-[2-(4-benzoxy-3-methoxyphenyl)isopropyl]benzamide}$ (VII), m. 165-7°; this results also from III and BzCl in cold dilute NaOH. VII (0.5 g.) and 0.8 g. POCl_3 in 2.7 cc. PhMe, refluxed 1 hr., give 0.45 g. 7-benzoxy-6-methoxy-1-phenyl-3-methyl-3,4-dihydroisoquinoline (VIII), m. 157-8.5°; picrate, yellow, m. 181-2.5°; methiodide, bright yellow, m. 215° (decomposition); HCl salt, m. 174-5° (decomposition). VIII (0.8 g.) and 7.5 cc. concentrated HCl in 7.5 cc. H_2O , heated 4 hrs. on the water bath, give 0.6 g. of the HCl salt, golden yellow, m. 206-7° (decomposition), of 7-hydroxy-6-methoxy-1-phenyl-3-methyl-3,4-dihydroisoquinoline (IX), cream, m. 103-5°; picrate, bright yellow, m. 223-5° (decomposition). I (0.3 g.) in 0.5 N NaOH, treated during 1 hr. with 1.1 g. PhCH_2COCl in 3.3 cc. C_6H_6 , gives 0.45 g. $\text{N-[2-(4-phenylacetoxymethoxyphenyl)isopropyl]phenylacetamide}$, m. 116-17°; with POCl_3 in CHCl_3 , 1.2 g. of the amide yields 0.42 g. 7-phenylacetoxymethoxy-1-benzyl-3-methyl-3,4-dihydroisoquinoline-HCl (X), m. 207-8° (decomposition); picrate, yellow, m. 165.5-6.5°; the free base becomes sticky on standing in the air and m. 60-70°; the base from 220 mg. X in 3 ml. MeOH, allowed to stand in an open vessel at room temperature for 14 days, gives 40 mg. of the 1-Bz analog, m. 144-5°; H_2SO_4 gives a yellow solution which becomes pale orange on warming; the Ac_2O solution develops a Prussian-blue color on boiling. X (0.7 g.) in 24 cc. 1:1 HCl, heated 2 hrs. on the water bath, gives 0.5 g. 7-hydroxy-6-methoxy-1-benzyl-3-methyl-3,4-dihydroisoquinoline-HCl (XI), pale green, m. 219-21°; picrolonate, buff-yellow, m. 233-4°; the free base, pale yellow, m. 98-107°, is oxidized in MeOH to the 1-Bz analog, pale yellow, m. 164-5° (HCl salt, pale yellow, m. 200-1° (decomposition)). $\text{N-[2-(4-Homoveratroyloxy-3-}$

methoxyphenyl)isopropyl]homoveratramide (a gum, 0.6 g.) and POCl_3 in CHCl_3 , refluxed in a H atmospheric for 1 hr., give 0.34 g. 7-homoveratroyloxy-6-methoxy-1-veratryl-3-methyl-3,4-dihydroisoquinoline, whose perchlorate, cream, m. 209-10°; picrolonate, ginger-brown, m. 190-1.5°; HCl salt, m. 201° (decomposition); hydrolysis with 1:1 HCl gives 7-hydroxy-6-methoxy-1-veratryl-3-methyl-3,4-dihydroisoquinoline- HCl (XII), very pale yellow, m. 210-11° (decomposition); picrolonate, orange-yellow, m. 178-9°. 7-Acetoxy-6-methoxy-1,3-dimethyl-3,4-dihydroisoquinoline (0.3 g.) and 0.14 g. Pd black, heated at 173-5° for 30 min. and the product hydrolyzed with 1:1 HCl , give 7-hydroxy-6-methoxy-1,3-dimethylisoquinoline (XII), m. 181-2° (picrate, deep yellow, m. 243° (decomposition)). VIII (0.2 g.) and 90 mg. Pd black, heated 1.5 hrs. at 170-5%/ 2 mm . give 85 mg. of the 7-benzoate, m. 140-1° (picrate, yellow, m. 210-11°), of 7-hydroxy-6-methoxy-1-phenyl-3-methylisoquinoline, m. 206-7° (picrate, lemon-yellow, m. 227°). The free base from X, heated with Pd black at 163-5%/ 2 mm . for 30 min. and hydrolyzed with 10% NaOH , gives 7-hydroxy-6-methoxy-1-benzyl-3-methylisoquinoline, m. 157-8°; the aqueous solution shows a deep green fluorescence; picrate, yellow, m. 199-200°. 7-Hydroxy-6-methoxy-1,3-dimethyl-1,2,3,4-tetrahydroisoquinoline, m. 169-70° (picrate, yellow-orange, m. 200-1° (decomposition)), results in 170-mg. yield from 0.1 g. of the dihydro derivative in 5 cc. dilute HCl with Pd -charcoal on shaking with H at 40° for 12 hrs. IX (50 mg.) yields 40 mg. of the HCl salt, m. 320° (decomposition), of 7-hydroxy-6-methoxy-1-phenyl-3-methyl-1,2,3,4-tetrahydroisoquinoline, m. 142-3.5°. XI (0.1 g.) with Pt oxide (12 hrs.) gives 85 mg. 7-hydroxy-6-methoxy-1-benzyl-3-methyl-1,2,3,4-tetrahydroisoquinoline- HCl , m. 243° (decomposition); the free base m. 118-19°; picrate, bright yellow, m. 230-1° (decomposition). VI (43 mg.) in 0.5 N HCl , shaken with Pt oxide and H for 3 hrs., gives 38 mg. 7-hydroxy-6-methoxy-3-methyl-1,2,3,4-tetrahydroisoquinoline, m. 151-2°. XII (68 mg.) gives 30 mg. 7-hydroxy-6-methoxy-1-veratryl-3-methyl-1,2,3,4-tetrahydroisoquinoline, m. 120-1°; dehydrogenation of 50 mg. with 30 mg. Pd black gives 30 mg. 7-hydroxy-6-methoxy-1-veratryl-3-methylisoquinoline, m. 173-4°; this base is isomeric with papaverine; both bases give a violet color on warming with H_2SO_4 .

IT 850857-64-6, 7-Isoquinolinol, 6-methoxy-3-methyl-1-phenyl-
(and derivs.)

RN 850857-64-6 HCPLUS

CN 7-Isoquinolinol, 6-methoxy-3-methyl-1-phenyl- (CA INDEX NAME)



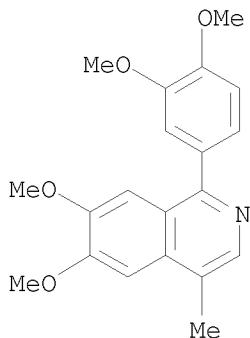
L13 ANSWER 295 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1942:581 HCPLUS
DOCUMENT NUMBER: 36:581
ORIGINAL REFERENCE NO.: 36:92h-i,93a-i,94a

TITLE: The synthesis of C-methyl derivatives of some medicaments. I, II
 AUTHOR(S): Sugasawa, Sigehiko; Sugimoto, Norio
 SOURCE: Yakugaku Zasshi (1941), 61, 62-8; Abstracts (in English) 26-30
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB Since C-Me derivs. are often less toxic than the original substances, S. and S. have introduced C-Me or vic-C-Me groups into well known medicaments in order to see their influence on the physiol. properties. Synthesis of 4-methyl- and 3,4-dimethylisoquinolines. Eupaverine and neupaverine are synthetic drugs having similar constitutions, resembling papaverine and have 1 Me group in the 3-position of the isoquinoline, skeleton. It has been attempted to synthesize compds. having 4-Me and 3,4-di-Me groups on the isoquinoline nucleus. As examples of the latter compds. partially hydrogenated phenanthridine and its analogs have already been synthesized by Sugasawa and his co-workers (C. A. 33, 4992.8; 34, 7291.8). The present synthesis of 4-methyl- and 3,4-dimethylisoquinoline proceeded according to the following scheme ($R = 3,4-(MeO)2C6H3$, $R' = H$ or Me):
 $RCOMe + BrCHR'CO2Et \rightarrow RC(OH)MeCHR'CO2Et \rightarrow RCMe:CR'COX$
 $\rightarrow RCHMeCHR'COX \rightarrow$
 $RCHMeCHR'NH2 \rightarrow RCHMeCHR'NHCOR \rightarrow (MeO)2C6H2.CHMe.CHR'.N:CR.fwdarw$
 $.(MeO)2C6H2.CMe:CR'.N:CR.$ (A) Synthesis of 1-substituted-6,7-dimethoxy-4-methylisoquinolines. Acetoveratrone and $BrCH_2CO_2Et$ by Reformatsky's reaction, followed by dehydration and saponification, gave β -methyl-3,4-dimethoxyhydrocinnamic acid (I). Heating of I and dry NH₃ gave the amide (II), plates, m. 126-7.5°. II and NaOCl gave 2-(3,4-dimethoxyphenyl)propylamine (III), b₁₀ 150-2°; HCl salt, platelets, m. 205° (from alc.-ether). III and veratroyl chloride in AcMe gave N-(3,4-dimethoxybenzoyl)-2-(3,4-dimethoxyphenyl)propylamine (IV), needles, m. 145° (from dilute alc.). Heating of IV, POC₁₃ and PhMe at 130° for 2 h. gave 1-(3,4-dimethoxyphenyl)-4-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline (V), (columns, m. 126-7°) (from EtOAc-petr. ether). The dehydrogenation of V according to Akabori (A. and Suzuki, C. A. 23, 4671) gave 1-(3,4-dimethoxyphenyl)-4-methyl-6,7-dimethoxyisoquinoline (VI), faintly yellow needles, m. 161-2°. N-Homoveratroyl-2-(3,4-dimethoxyphenyl) propylamine, (VII), scales, m. 172.5° (from alc.), was prepared by the same method used for IV. 1-(3,4-Dimethoxybenzyl)-4-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline (VIII) was prepared by the same method used for V. Since it was difficult to crystallize, it was identified as the picrate, yellow needles, m. 103° (from alc.-ether). (B) Synthesis of 3,4-dimethylisoquinoline derivs. The methods of preparation are essentially the same as those given in the foregoing section. α,β -Dimethyl-3,4-dimethoxyhydrocinnamide, platelets, m. 136° (from H₂O). 1,2-Dimethyl-2-(3,4-dimethoxyphenyl)-ethylamine, b₉ 152-3°; HCl salt, platelets, m. 202-3° (from alc.-ether). N-(3,4-Dimethoxybenzoyl)-1,2-dimethyl-2-(3,4-dimethoxyphenyl)ethylamine, needles, m. 121-2° (from EtOAc-petr. ether). 1-(3,4-Dimethoxyphenyl)-3,4-di-Me-6,7-dimethoxy-3,4-dihydroisoquinoline, columns, m. 84-7° (from EtOAc-petr. ether); HCl salt, yellow crystalline powder, m. 206-7° (from alc.-ether).

Picrate, yellow grains, m. 186-7.5° (from absolute alc.-ether).
 1-(3,4-Dimethoxyphenyl)-3,4-dimethyl-6,7-dimethoxyisoquinoline, light yellow needles, m. 159-60° (from PhH-petr. ether). (C) Synthesis of dimethylcocaine. Heating of acrylic acid and 2,3-dimethylbutadiene at 180° for 10 h. gave 3,4-dimethyl-1,2,5,6-tetrahydrobenzoic acid (IX), m. 72-4°, b4 122-4°. Dehydrogenation of IX by heating with S at 200-220° gave 3,4-dimethylbenzoic acid (X), prisms, m. 163°. X and SO₂Cl gave the corresponding acid chloride (XI), b12 124-7°. Heating of XI and ecgonine Me ester in xylene for 2 h. gave dimethylcocaine, columns, m. 92°, [α]D19 - 18.02° (in MeOH); HCl salt, m. 193° (decomposition). (D) Synthesis of 3,4-dimethylcinnamoyl-p-hydroxyphenylurea. Treating of 3,4-Me₂C₆H₃COCl by Rosemund's method gave 3,4-dimethylbenzaldehyde (XII), b11 101°; semicarbazone, m. 228°. XII, malonic acid, pyridine and a drop of piperidine gave 3,4-dimethylcinnamic acid (XIII), needles, m. 172°.

The literature gives the m. p. as 142°, but this is erroneous, since the product obtained by another method m. 172°. The acid chloride of XIII and p-hydroxyphenylurea in pyridine gave 3,4-dimethylcinnamoyl-p-hydroxyphenylurea, needles, m. 206°. (E) Synthesis of 4,5-dimethyl-N,N,N',N'-tetraethylphthalamide. Heating of 4,5-dimethyl-1,2,3,6-tetrahydronaphthalic anhydride and S at 240° for 2 h. gave 4,5-dimethylphthalic anhydride (XIV), m. 206°. XIV and NHEt₂ gave 4,5-dimethyl-N,N-di-ethylphthalamic acid (XV), platelets, m. 167° (from PhH). XV and SOCl₂ were heated at 80° for 0.5 h. After the excess of SOCl₂ was evaporated off, the residue in AcMe was added to NHEt₂ in AcMe. The NHEt₂.HCl was filtered off and the solvent was evaporated. On recrystn. from ligroin, crystals of 4,5-dimethyl-N,N,N',N'-tetraethylphthalamide, m. 62°, were obtained.

IT 20225-95-0P, Isoquinoline,
 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-4-methyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 20225-95-0 HCPLUS
 CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-4-methyl- (CA INDEX NAME)



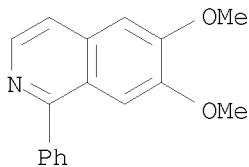
L13 ANSWER 296 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1940:24257 HCPLUS
 DOCUMENT NUMBER: 34:24257

ORIGINAL REFERENCE NO.: 34:3747a-f
 TITLE: The synthesis of spasmolytic isoquinoline bases. Some new reversible N-O acyl migrations
 AUTHOR(S): Vinkler, Elemer; Bruckner, Gyozo, Jr.
 SOURCE: Magyar Chemiai Folyoirat (1939), 45, 147-55
 CODEN: MGCFVA; ISSN: 0368-9808
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Treating $3,4-(\text{MeO})_2\text{C}_6\text{H}_3\text{CH}(\text{OH})\text{CH}(\text{NO}_2)\text{Me}$ (I) in pyridine with BzCl and evaporating the ether extract of the resulting crystalline mass gave a greenish oil identified as α -(3,4-dimethoxyphenyl)- α -benzoyloxy- β -nitropropane (II). The reaction of I in pyridine with anisoyl chloride and purification of the CHCl_3 extract of the product led to an olive-green oil consisting of the α -anisoyloxy analog (III) of II. Treating I in pyridine with freshly prepared veratroyl chloride, preparing a CHCl_3 extract and then evaporating this extract gave a greenish oil consisting of the α -veratroyloxy compound (IV). Dissolving I in a mixture of pyridine and CHCl_3 and adding freshly distilled PhCH_2COCl in CHCl_3 , then preparing a CHCl_3 extract and evaporating it in vacuo gave a yellow oil consisting of the α -phenacetoxy compound (V). Electrolytic reduction of the II using Pb electrodes in 20% H_2SO_4 (anolyte) and the alc. solution of the compound (catholyte) gives colorless needles of α -(3,4-dimethoxyphenyl)- β -benzoylaminopropanol, m. 136° . The electrolytic reduction of III led to colorless needles of the β -anisoyl amino compound, m. 137° . Similar treatment of IV gave also colorless needle crystals of the β -veratroyl amino compound, m. $155-6^\circ$. Electrolytic reduction of V gave an oily product consisting of the β -phenylacetyl amino compound (VI). Treating VI in purified xylene with POCl_3 and adding concentrated NaOH to the cooled solution gave white needles with silky luster which lost their water of crystallization at 65° when heated in vacuo, m. 104° and were identified as 1-benzyl-3-methyl-6,7-dimethoxyisoquinoline. Into veratraldehyde and MeNO_2 in absolute alc., dilute alc., NaOMe was dropped with cooling to the solution. The crystalline mass gave, after drying, a white powder consisting of Na α -(3,4-dimethoxyphenyl)- β -aci-nitroethanol (VII). VII in CHCl_3 suspension was treated with BzCl in CHCl_3 . After filtering the precipitated NaCl and evaporating the filtrate a reddish thick oil consisting of α -(3,4-dimethoxyphenyl)- α -benzoyloxy- β -nitroethane (VIII) was obtained. The electrolytic reduction of VIII lead to crude α -(3,4-dimethoxyphenyl)- β -benzoylamin ethanol (IX). IX in toluene was mixed with POCl_3 and heated, then cooled, shaken out with dilute HCl and made alkaline with NaOH with cooling. After purifying the solution picric acid was added to form the picrate, m. 250° , of 1-phenyl-6,7-dimethoxyisoquinoline.

IT 857806-32-7P, Isoquinoline, 6,7-dimethoxy-1-phenyl-, picrate
 RL: PREP (Preparation)
 (preparation of)
 RN 857806-32-7 HCPLUS
 CN Isoquinoline, 6,7-dimethoxy-1-phenyl-, picrate (3CI) (CA INDEX NAME)

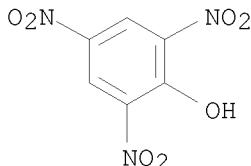
STN

CRN 4029-09-8
CMF C17 H15 N O2



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



L13 ANSWER 297 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1940:15418 HCPLUS
DOCUMENT NUMBER: 34:15418
ORIGINAL REFERENCE NO.: 34:2383b-i,2384a-h
TITLE: Alkaloid-like compounds from brazilin and hematoxylin
AUTHOR(S): Pfeiffer, P.; Breitbach, J.; Scholl, W.
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1940)
, 154, 157-208
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Through a series of simple reactions brazilin and hematoxylin may be converted into alkaloid-like compds. which are closely related to papaverine and laudanosine. Hematoxylin is methylated and oxidized to tetramethylhematoxylonone, which is reduced by Mg and AcOH to tetramethylhematoxylonol (I) (C. A. 32, 4597.7); oxime (II), C₂₀H₂₃O₇N, m. 223° (decomposition); the halochromy of II is wine-red, with a blue-lilac filtrate; HCl in MeOH gives I. Heating 20 g. I and 8 g. NH₂OH·HCl with 10 g. KOH in 100 cc. EtOH for 4 hrs. on the water bath, pouring into 400 cc. H₂O, neutralizing with AcOH and crystallizing the crude product (20 g.) from EtOH or C₆H₆ gives anhydrotetramethylhematoxylonol oxime [1-(2'-hydroxy-3',4'-dimethoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline oxide] (III), C₂₀H₂₁O₆N, leaflets, m. 220°; III also results on heating II in EtOH with alkali; it also crystallizes as long needles, m. 191-2°, changing after several days to the stable form; the presence of a phenolic HO group is indicated by the solubility

of III in cold dilute NaOH and its precipitation by CO₂; 4 of the O atoms are present as MeO groups; the 6th O atom is in the form of a N:O group, as shown by the formation of VI with SO₂ in AcOH. III (1 g.) and 1 g. MeI in 2.5 g. NaOH in 50 cc. H₂O, refluxed 6 hrs., give 0.4 g. of the methiodide (IV), C₂₂H₂₆O₅NI, yellow, m. 227-8°; IV results in a nearly quant. yield by heating 1 g. I and 5 cc. MeI with 25 cc. NaOH in 50 cc. H₂O and 40 cc. EtOH for 15 hrs. and then passing CO₂ through the boiling solution for 3 hrs. In this reaction the phenolic HO group is methylated and the N:O group is transformed into NMeI. Heating III and Me₂SO₄ in C₆H₆, removing the C₆H₆, dissolving the residue in H₂O and adding saturated KI in H₂O, give the methiodide (V) of III, C₂₁H₂₄O₆NI, which seps. from a dilute MeOH solution in the dark as light yellow crystals, m. 206-8°, sensitive to light; in this reaction the N:O group is changed to NOMEI. The picrate of III, grayish yellow, m. 216-17° (decomposition). Addition of 5 g. Zn in portions to 10 g. III in 50 cc. hot AcOH and allowing the mixture to stand 12 hrs. at room temperature give the desoxoanhydro compound [1-(2'-hydroxy-3',4'-dimethoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline] (VI), m. 174°; H₂SO₄ causes no halochromy; in this reaction the O of the N:O group is split off; ClCH₂CH₂OH in MeOH gives a decided brown color in 30 min.; without the MeOH the color appears in 9 hrs. (test for an epichlorohydrin). VI in hot HCl or dry HCl in C₆H₆ gives the HCl salt, decomp. 230-5°; picrate, yellow, m. 210°. VI and Me₂SO₄ in C₆H₆ give the methosulfate, m. 168-70°; KI gives the methiodide (VII), pale yellow, m. 230-1°, which also results from VI and MeI in CHCl₃. Warming 1 g. VI and 1 g. AcONa in 15 cc. Ac₂O for 1 hr. on the water bath gives the acetate, m. 174° (hydrate, m. 86-8°; picrate, light yellow, m. 202-3°; methiodide, with 1 mol. H₂O, pale yellow, m. 118°). VI and Me₂SO₄ in 5% NaOH give the Me ether [1-(2',3',4'-trimethoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline] (VIII), m. 129-30°; picrate, golden yellow, m. 185-6°; the methiodide, yellow, m. 227-8°, results from VI and MeI in MeOH-NaOH, from MeI in CHCl₃, followed by MeI in NaOH, or from VIII and MeI in CHCl₃. Reduction of III or VI with Na in boiling EtOH gives 1-(2-hydroxy-3',4'-dimethoxyphenyl)-3-methyl-6,7-dimethoxytetrahydroisoquinoline, C₂₀H₂₅O₅N, m. 181-4°; picrate, yellow or red, with 1 mol. H₂O, m. 175-8°; light transforms the yellow into the red form. VII, transformed into the methochloride and reduced with Zn in HCl, gives the N-methyltetrahydro derivative, which could not be crystallized but was analyzed as the picrate, light yellow, m. 190°. Oxidation of VI with alkaline KMnO₄ gives metahemipinic acid, 3,4,1,2-(MeO)₂C₆H₂(CO₂H)₂, identified as the ethylimide, m. 228°. With HNO₃ VI gives an acid (IX), whose picrate, yellow, with 1 mol. H₂O or MeOH, decomp. 240°; the Me ester of IX forms a picrate, yellow, m. 212°. Trimethylbrazilonol (X) oxime, warmed with KOH in C₅H₅N or EtOH for 0.5 hr., or X, NH₂OH.HCl, KOH and EtOH refluxed 4 hrs., give the anhydro compound [1-(2'-hydroxy-4'-methoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline oxide] (XI), m. 243°; HCl salt, m. 131° (decomposition); Bz compound, m. 176°; the Me ether could not be crystallized; its picrate m. 180-5°; HCl salt, decomp. 115°. Reduction of XI with Zn or SO₂ in hot AcOH gives the desoxoanhydro compound, 1-(2'-hydroxy-4'-methoxyphenyl)-3-methyl-6,7-dimethoxyisoquinoline (XII), m. 188-9°; picrate, orange-yellow, m. 224-5°; methiodide, with 1.33 mols. H₂O, m. 207-8°. The Me ether (XIIA) of XII m. 110°; it was purified through the picrate, m. 212-15°; methosulfate, m. 170°; methiodide, with 0.5 mol. H₂O, yellow, m. 170°. Dimethyl-β-resorcylic acid with PCl₅ or SOCl₂ gives the

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chloride (XIII), m. 54-6°; amide, m. 132°; anilide, m. 141°. α -(3,4-Dimethoxyphenyl)- β -aminopropanol (XIV), m. 128-9°, results from hydrolysis of the Ac derivative (Bruckner, C. A. 29, 5825.6). Condensation of XIII and XIV in C6H6 gives 96% of the acylamide, 3,4-(MeO)2C6H3CH(OH)CHMeNHCOC6H3(OMe)2-2,4, pale yellow resin; ring closure with POCl3 in PhMe gives 1-(2',4'-dimethoxyphenyl)-3-methyl-7,8-dimethoxyisoquinoline, m. 144-5° (crude yield, 76.8%); picrate, deep yellow, m. 232-5°; methosulfate, m. 239°; methiodide, yellow, m. 217-19° (decomposition); the tetrahydro derivative yields a picrate, deep golden yellow, m. 203-5°. The isomeric XIIA could not be detected by fractional crystallization of the crude base or its picrate or by chromatographic fractionation from C6H6 on Al2O3. 2,4-HO(MeO)C6H3CO2H with PhNMe2 and ClCO2Et in C6H6-Et2O gives the 2-carbethoxy derivative, m. 111° (decomposition); the chloride (XV) is a yellow oil; anilide, m. 215°. Condensation of XV and XIV in C5H5N-C6H6 gives the amide, 3,4-(MeO)2C6H3CH(OH)CHMeNHCOC6H3(OCO2Et)OMe-2,4, a yellow resin; ring closure yields 1-(2'-hydroxy-4'-methoxyphenyl)-3-methyl-7,8-dimethoxyisoquinoline, whose yellow picrate decomp. 272-5°. XIV and 2,3,4-(MeO)3C6H2COCl give the amide, 3,4-(MeO)2C6H3CH(OH)CHMeNHCOC6H2(OMe)3-2,3,4, m. 127-8°; ring closure gives 94% of 1-(2',3',4'-trimethoxyphenyl)-3-methyl-7,8-dimethoxyisoquinoline, m. 110-12°; picrate, yellow, m. 183-4°; methosulfate, m. 225-7°; methiodide, pale yellow, m. 226-7° (decomposition). Thus, in no case was a synthetic product obtained which was identical with those prepared from the natural compds.

IT 855650-20-3P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Alkaloid-like compounds from brazilin and hematoxylin)

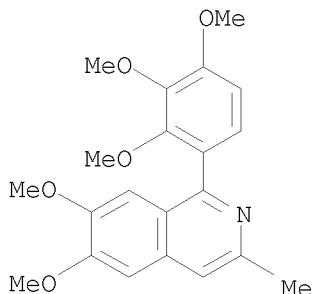
RN 855650-20-3 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-3-methyl-1-(2,3,4-trimethoxyphenyl)-, picrate
(5CI) (CA INDEX NAME)

CM 1

CRN 20226-00-0

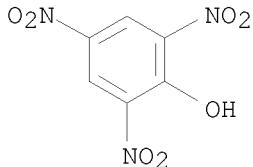
CMF C21 H23 N 05



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L13 ANSWER 298 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1939:64749 HCPLUS

DOCUMENT NUMBER: 33:64749

ORIGINAL REFERENCE NO.: 33:9307e-i

TITLE: Synthesis of compounds related to papaverine. VI.
Synthesis of 3-methylisoquinoline derivatives

AUTHOR(S): Sugasawa, Sigeiko; Kakemi, K.

SOURCE: Yakugaku Zasshi (1937), 57, 172-80 (in English, 24-7)

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

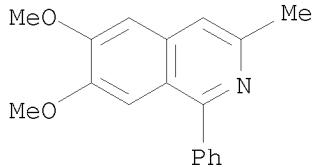
LANGUAGE: Unavailable

AB The synthesis of methylisoeugenol pseudonitrosite, α -(3,4-dimethoxyphenyl)- β -nitrosopropanol Me ether and α -(3,4-dimethoxyphenyl)- β -aminopropanol Me ether-HCl (I) was carried out according to Bruckner (C. A. 29, 5825.6, 5826.6). Benzoylation of 5 g. I gave N-benzoyl- α -methyl- β -methoxy- β -(3,4-dimethoxyphenyl)ethylamine (II), C₁₉H₂₃NO₄, m. 121° (yield 90%). II (2 g.) in 30 cc. anhydrous xylene and 11 cc. POC₁₃ when heated for 30 min. on the oil bath gave 1-phenyl-3-methyl-6,7-dimethoxyisoquinoline, C₁₈H₁₇NO₂, m. 128° (yield 60%); HCl salt, decomposing 245°. The Na salt of 4-hydroxy-3,5-dimethoxy-1-allylbenzene (prepared according to Hahn and Wassmuth, C. A. 28, 4047.3) and 120 g. 40% KOH in AmOH when heated on the oil bath at 140° for 20 hrs. gave 20 g. oily 4-hydroxy-3,5-dimethoxy-1-propenylbenzene, which on methylation gave isoelemicin (III), b₆ 145-7° (yield 95%). III (8.7 g.) in 65 cc. ether, NaNO₂ solution and 38 cc. 20% H₂SO₄ gave isoelemicin pseudonitrosite (yield 90%). The nitrosite (5 g.) by the usual procedure gave nitroisolemicin (IV), C₁₂H₁₅NO₅, m. 94° (yield 64%). IV (14.3 g.) in 60 cc. absolute MeOH when treated with NaOMe gave α -(3,4,5-trimethoxyphenyl)- β -nitropopropanol Me ether, C₁₃H₁₉NO₆, m. 86° (yield 94%), which on reduction gave the β -amino compound (V), b_{4.5} 153-4° (yield 71%) (HCl salt, C₁₃H₂₂O₄NCl, m. 197°). Benzoylation of 3.6 g. V gave N-benzoyl- α -methyl- β -methoxy- β -(3,4,5-trimethoxyphenyl)ethylamine, C₂₀H₂₅NO₅, m. 157.5-8° (yield 94%), which when treated with POC₁₃ gave 1-phenyl-3-methyl-6,7,8-trimethoxyisoquinoline, C₁₉H₁₉NO₃, m. 117° (yield 80%); HCl salt, decomposing 180-1°. V (2.5 g.) in 20 cc. 10% Na₂CO₃ and 2.3 g. trimethylgalloyl chloride in 5 cc. absolute acetone gave a compound (4.7 g.), which when treated with POC₁₃ gave 1-(3',4',5'-trimethoxyphenyl)-3-methyl-6,7,8-trimethoxyisoquinoline-HCl, C₂₂H₂₆O₆NCl, decomposing 197.5° (yield 90%).

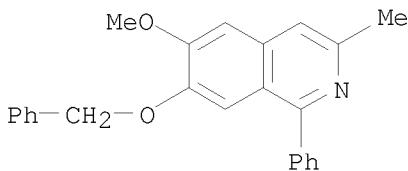
IT 20225-88-1P, Isoquinoline, 6,7-dimethoxy-3-methyl-1-phenyl-
RL: PREP (Preparation)

STN

(preparation of)
RN 20225-88-1 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-3-methyl-1-phenyl- (CA INDEX NAME)



L13 ANSWER 299 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1938:38828 HCAPLUS
DOCUMENT NUMBER: 32:38828
ORIGINAL REFERENCE NO.: 32:5402i,5403a-c
TITLE: Synthesis of nitrogen-ring compounds. XI. Synthesis of isoquinoline derivatives. 8. Synthesis of benzeneazoquinoline derivatives
AUTHOR(S): Sugasawa, Shigehiko
SOURCE: Yakugaku Zasshi (1938), 58, 265-8
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 32, 4161.5. Isoeugenol (4.2 g.) in MeOH, 17 g. K₂CO₃ and 32 g. PhCH₂Cl when heated on the water bath for 5 hrs. gave o-benzyliseugenol, b5 198-204°, m. 46-52° (71% yield), which gave benzylisoeugenol pseudonitrosite (I), m. 105-8° (80% yield). I (30 g.) when treated with 10 g. KOH in the sealed container for 8 hrs., followed by H₂SO₄ to make it slightly acid, gave β-nitro-o-benzylisoeugenol (II), C₁₇H₁₇O₄N, m. 89-90° (90% yield). II (9.3 g.) in 90 cc. MeOH when heated with 2 g. Na in 130 cc. MeOH gave 1 - (β-nitro-α-methoxypropyl)-3-methoxy-4-benzyloxy-benzene (III), C₁₈H₂₁O₅N, m. 115-16° (93% yield). Reduction of III (either catalytic or electrolytic reduction) gave an amine (83% yield), which on benzylation gave the N-Bz derivative(IV), C₂₅H₂₇O₄N, m. 165-6° (50% yield). IV (3 g. in 30 cc. toluene and 9 g. POCl₃) when treated on the oil bath for 30 min. gave 1-phenyl-3-methyl-6-methoxy-7-benzyloxyisoquinoline (V), C₂₄H₂₁O₂N, m. 134° (1.7 g. yield), which gave 1-phenyl-3-methyl-6-methoxy-7-hydroxyisoquinoline (VI), C₁₄H₁₅O₂N, m. 186°, the HCl salt decomposing 140-50°. VI (0.5 g.), 1.2 cc. KOH, 1 g. Na₂CO₃ in 20 cc. water and PhN₂Cl gave 1-phenyl-3-methyl-6-methoxy-7-hydroxy-8-benzeneazoisoquinoline, C₂₃H₁₉N₃O₂, decomposing 205-7°.
IT 102664-48-2P, Isoquinoline,
7-(benzyloxy)-6-methoxy-3-methyl-1-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 102664-48-2 HCAPLUS
CN Isoquinoline, 6-methoxy-3-methyl-1-phenyl-7-(phenylmethoxy)- (CA INDEX NAME)



L13 ANSWER 300 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1938:24334 HCPLUS

DOCUMENT NUMBER: 32:24334

ORIGINAL REFERENCE NO.: 32:3403i,3404a-g

TITLE: Synthesis of spasmolytically active
3-methylisoquinolines

AUTHOR(S): Bruckner, Viktor; von Fodor, Gabor

SOURCE: Berichte der Deutschen Chemischen Gesellschaft
[Abteilung] B: Abhandlungen (1938), 71B,
541-9

CODEN: BDCBAD; ISSN: 0365-9488

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB The method of synthesizing isoquinoline bases of the type (C. A. 30, 5990.9), where R = PhCH₂, 3,4-(MeO)2C₆H₃CH₂, 3,4-CH₂O₂C₆H₃CH₂, Ph, and 3,4-CH₂O₂C₆H₃, has been extended to the compds. where R = p-MeOC₆H₄, 3,4-(MeO)2C₆H₃ and 3,4,5-(MeO)3C₆H₂, and analogous derivs. of I with 2 MeO groups instead of the CH₂O₂ grouping on the left side of the formula above. The object of the work was not only to show that the method is capable of quite wide application but also to secure further exptl. material for determining the relation between structure and spasmolytic activity. A new observation made was that the acylation of the intermediate ArCH(OH)CH(NH₂)Me (II) present in solution can best be effected at 40-50°; the resulting crude products can be condensed directly by means of POC₁₃ in toluene or xylene. The method has the following advantages over other methods of synthesizing 3-methylisoquinolines: (1) the ring closure gives the isoquinoline derivative directly so that the dehydrogenation with Pd is avoided; (2) the II or their salts need not be isolated but can be converted into their stable acyl derivs. and further worked up; (3) the propenylphenol ethers used as the starting materials are relatively cheap. All of the I showed on the isolated intestinal strip a spasmolytic action which in general was not only equal to that of papaverine but even surpassed it considerably. Some were also superior, as regards quality of action and toxicity, to the analogous compds. demethylated at position 3 and to papaverine. Of special practical interest was the question whether the homoaryl residue (R) could be replaced by aryl residues without damage to the pharmacol. properties, for the BzOH derivs. required for the introduction of such aryl residues are in general considerably cheaper than the corresponding ArCH₂CO₂H derivs. The results obtained indicate that the presence of a CH₂ group between the heterocyclic and the aromatic ring is by no means necessary for pharmacol. activity. The following compds. are described.

α -3,4-Methylenedioxyphenyl- β -acylaminopropanols: anisoyl (1.2 g. from 1.5 g. of the β -NH₂ compound and MeC₆H₄COCl), m. 179°; veratroyl (almost quant.), m. 158°; 3,4,5-trimethoxybenzoyl (almost quant.), m. 119-20°. α - 3,4 - Dimethoxyphenyl - β -

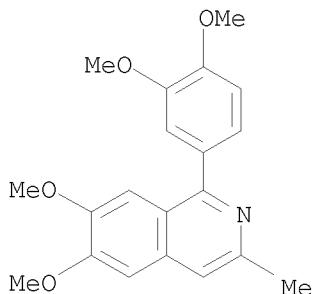
STN

acylaminopropanols: phenacetyl (yield not very abundant), m. 116°; homoveratroyl, m. 142°; homopiperonoyl, m. 156°; benzoyl, m. 136°; anisoyl, m. 137°; veratroyl, m. 156°; piperonoyl, m. 148°; 3,4,5-trimethoxybenzoyl, m. 159°; 3,4,5-triethoxybenzoyl, needles with 1 MeOH lost in vacuo at 50°, m. 75°. 1-Aryl-3-methyl-6,7-methylenedioxyisoquinolines: 4-methoxyphenyl, isolated as the HCl salt, crystals with 1 H₂O, m. 180°; 3,4-dimethoxyphenyl, m. 160-1°; 3,4,5-trimethoxyphenyl, m. 152-3°.

1-Aryl-3-methyl-6,7-dimethoxyisoquinolines: phenyl, m. 128° (HCl salt, m. 245° (decomposition)); 4-methoxyphenyl, isolated as the HCl salt, faintly yellow, m. 185° (decomposition); 3,4-dimethoxyphenyl, m. 143° (HCl salt, m. 193°); 3,4-methylenedioxyphenyl, m. 186° (HCl salt, greenish, m. 190-1° (decomposition)); 3,4,5-trimethoxyphenyl, m. 186° (HCl salt, m. 122°); 3,4,5-triethoxyphenyl, m. 122° (HCl salt, greenish, m. 201°); benzyl, m. 106° (HCl salt, crystals with 1 H₂O, m. 204°); 3,4-dimethoxybenzyl, m. 136°; 3,4-methylenedioxybenzyl, m. 129°.

IT 17340-97-5P, Isoquinoline,
1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl-
RL: PREP (Preparation)
(preparation of)

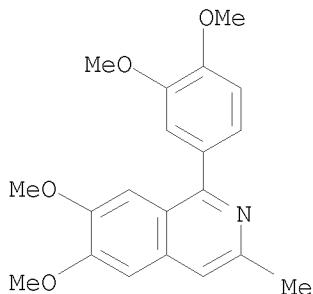
RN 17340-97-5 HCPLUS
CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



L13 ANSWER 301 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1938:942 HCPLUS
DOCUMENT NUMBER: 32:942
ORIGINAL REFERENCE NO.: 32:171i,172a-b
TITLE: Spectrographic investigation in the isoquinoline series
AUTHOR(S): Gerendas, M.; Varga, Eva
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1937), 149, 175-82
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB In the ring closure of α -piperonyl- α -hydroxy- β -N-piperonoylaminopropane (I) to neupavarine (1-piperonyl-3-methyl-6,7-methylenedioxyisoquinoline (II), an intermediate product with 1 mol H₂O

less than I and 1 mol H₂O more than II was isolated, which was believed to be 1-piperonyl-3-methyl-3,4-dihydro-4-hydroxy-6,7-methylenedioxyisoquinoline (III) (Bruckner and Kr. acte. amli, C. A. 30, 5990.9). The structure of III has been investigated spectrog. The following values of λ maximum in m μ are given for the 3 maximum I, II and III: I, -, 291, 261; α -veratryl analog of I, -, 287, 261; α -veratryl- α -hydroxy- β -N-veratroylaminopropane, -, 281, 258; α -piperonyl- α -hydroxy- β -N-acetylaminopropane, -, 286, 234; α -anisyl analog -, 275, 225. II, 336, 289, 240; 1-piperonyl-3-methyl-6,7-dimethoxyisoquinoline, 334, 288, 242; 1-veratryl analog, 334, 287, 240; 1,3-dimethyl-6,7-methylenedioxyisoquinoline, 329, 280, 238; 6,7-di-MeO analog, 325, 278, 237. III, -, 286, 232; α -piperonyl- α -hydroxy- β -N-homopiperonylaminopropane, -, 286, 236. Curves are given for all these compds. The structure of III is confirmed by these results.

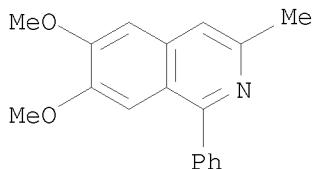
IT 17340-97-5P, Isoquinoline,
1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl-
RL: PREP (Preparation)
(preparation of)
RN 17340-97-5 HCAPLUS
CN Isoquinoline, 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3-methyl- (CA INDEX NAME)



L13 ANSWER 302 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1937:45471 HCAPLUS
DOCUMENT NUMBER: 31:45471
ORIGINAL REFERENCE NO.: 31:6335a-c
TITLE: Relation between the surface activity and the spasmolytic effect on smooth muscles
AUTHOR(S): Szende, Jolan; Telbisz, Martha
SOURCE: Magyar Gyogyszeresztudomanyi Tarsasag Ertesitoje (1937), 13, 449-53
CODEN: MGGTAP; ISSN: 0368-9859
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB For alkaloids of the papaverine type
(homoveratryl-3-methyl-6,7-methylenedioxyisoquinoline,
1-phenyl-3-methyl-6,7-dimethoxyisoquinoline,
1-phenyl-3-methyl-6,7-methylenedioxyisoquinoline,
1-benzyl-3-methyl-6,7-methylenedioxyisoquinoline,
1-piperonyl-3-methyl-6,7-methylenedioxyisoquinoline (Neuparverin Merck),
1,3-dimethyl-6,6-methylenedioxyisoquinoline,

STN

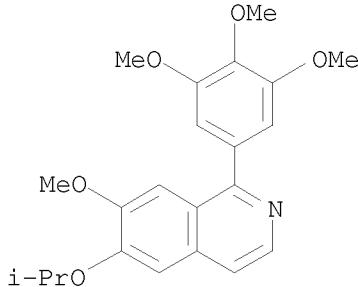
2- β -aminoethyl-5,6-dimethoxybenzoic acid) the spasmolytic effect is proportional to surface activity determined by the method of DuNouy-Brinkmann.
IT 20225-88-1P, Isoquinoline, 6,7-dimethoxy-3-methyl-1-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 20225-88-1 HCAPLUS
CN Isoquinoline, 6,7-dimethoxy-3-methyl-1-phenyl- (CA INDEX NAME)



L13 ANSWER 303 OF 310 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1936:19541 HCAPLUS
DOCUMENT NUMBER: 30:19541
ORIGINAL REFERENCE NO.: 30:2572a-e
TITLE: Syntheses in the papaverine group. IV. Synthesis of 1 - (3',4',5' - trimethoxyphenyl) - 6 - propoxy - 7 - methoxyisoquinoline
AUTHOR(S): Sugasawa, Shigehiko; Kakemi, Kiichiro
SOURCE: Yakugaku Zasshi (1935), 55, 1283-8; Abstracts 244-7
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. C. A. 29, 5116.6. Isovaniillin (30.4 g.) in 10% alc. KOH (1.2 mols.) on heating for 4 hrs. on the water bath with PrBr or iso-PrBr (29.6 g.) gave, resp., 3-propoxy-4-methoxybenzaldehyde (I) (yield, 32-4 g.), b4 156-8°, m. 51°, and iso-Pr derivative, b2 132-4°. I (2.9 g.), galloylglycine tri-Me ether (4 g.), dry NaOAc (2 g.) and anhydrous AcOH (7 cc.) on heating on the water bath for 1 hr. gave 2 - (3',4',5' - trimethoxyphenyl) - 4 - (3' - propoxy - 4' - methoxybenzal)-5-oxazolone (II), m. 172°, and iso-Pr derivative, m. 188d°. II (12.8 g.) in MeOH (65 cc.) and a small amount of Na2CO3 on heating on the steam bath for 4 hrs. gave a clear yellow solution which on addition of 10% MeOH-KOH (25 cc.), followed by further heating for 1 hr. longer, gave α -galloylamino-3-propoxy-4-methoxycinnamic acid tri-Me ether (III), m. 213°, and iso-Pr derivative, m. 137.5°. III (8.9 g.), quinoline (30 cc.) and Cu chromite (0.9 g.) on heating on the water bath for 15 min. at 160-190°, gave ω -galloylamino - 3 - propoxy - 4 - methoxystyrene tri - Me ether (IV), m. 133°, and iso-Pr derivative, m. 137.5°. Reduction of IV catalytically with PtO2-Pt black gave galloyl β -(3-propoxy-4-methoxy-phenyl)ethylamide tri-Me ether (V), m. 109°, and iso-Pr derivative, m. 102°. V (2 g.) in dry CHCl3 (20 cc.) was kept at room temperature for 3-4 days with powdered PC15 (4 g.); the yellow crystals which separated were 1 -(3',4',5' - trimethoxyphenyl)-6-propoxy-7-methoxy-3,4-dihydroisoquinoline-HCl, m. 208-9° (free base, m. 104°), and iso-Pr derivative-HCl, m. 217-18° (free base, m. 96-7°). The dehydrogenation of the above compds. gave corresponding

STN

1-(3',4',5'-trimethoxyphenyl)-6-propoxy-7-methoxyisoquinoline, m.
208-9°, and iso-Pr derivative, m. 199°.
IT 857805-10-8P, Isoquinoline,
6-isopropoxy-7-methoxy-1-(3,4,5-trimethoxyphenyl)-
RL: PREP (Preparation)
(preparation of)
RN 857805-10-8 HCPLUS
CN Isoquinoline, 7-methoxy-6-(1-methylethoxy)-1-(3,4,5-trimethoxyphenyl)-
(CA INDEX NAME)



L13 ANSWER 304 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1935:39359 HCPLUS
DOCUMENT NUMBER: 29:39359
ORIGINAL REFERENCE NO.: 29:5116f-i,5117a-b
TITLE: Synthesis of papaverine derivatives. II. Synthesis of
1 - (3',4',5' - trimethylphenyl) - 6,7 -
diethoxyisoquinoline
AUTHOR(S): Sugasawa, Shigebiko
SOURCE: Yakugaku Zasshi (1935), 55, 224-33;in
English 58-63
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 29, 169.3. Veratrahippuric acid (10 g.) in quinoline (40 cc.)
and Cu chromite (1 g.) on heating gradually on the oil bath at
120-80° for 20 mins. gave 3,4-dimethoxy- ω -benzamidostyrene
(I), C17H17O3N, m. 138°, colorless needles. Reduction of I
catalytically in AcOH gave- β -(3,4-dimethoxyphenyl)ethylbenzamide
(II), C17H19O3N, m. 90°, which did not depress the m. p. of the
product obtained by benzoylating 3,4-(MeO)2C6H3CH2CH2NH2. II (5 g.) in
toluene (30 cc.) and POCl3 (15 g.) on boiling for 2 hrs. gave
1-phenyl-6,7-dimethoxy-3,4-dihydroisoquinoline (III), C17H17O2N, m.
120-1° (yield 4 g.). Aminoacetonitrile sulfate (5 g.) in excess 5%
NaOH on treating with galloyl chloride tri-Me ether (7 g.) gave
galloylglycinonitrile tri-Me ether (IV), C12H14O4N2, m. 186-7°
(yield 6-6.5 g.). IV (10 g.) in absolute alc. (50 cc.) and concentrated H2SO4
(10 g.) on refluxing on the steam bath for 1 hr. gave Et galloylglycine tri-Me
ether (V), C14H19O6N, m. 109°, colorless needles. Hydrolysis of V
with alc. KOH gave galloylglycine tri-Me ether (VI), C12H15O6N, m.
218°, colorless scales. 3,4-(EtO)2C6H3CHO (8 g.), VI (10 g.),
fused NaOAc (5 g.) and Ac2O (20 cc.) on heating on the steam bath for 1

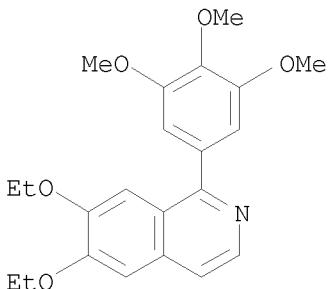
hr. gave 2-(3',4',5'-trimethoxyphenyl)-4-(3',4'-diethoxybenzal)oxazolone (VIII), C₂₃H₂₅O₇N, m. 163-4° (yield 10-11 g.). VII (10 g.) in 5% NaOH (300 cc.) on boiling for 3 hrs. gave 3',4'-diethoxybenzal-3,4,5-trimethoxyhippuric acid (VIII), C₂₃H₂₇O₈N, m. 220-1°, colorless needles. VIII (7 g.) in quinoline (21 cc.) and Cu chromite (0.7 g.) on heating, on the oil bath at 180-90° for 20 mins. gave ω -galloylamido-3,4-diethoxystyrene tri-Me ether (IX), C₂₂H₂₇O₆N, m. 157-8°, colorless long needles. Catalytic reduction of IX gave N'-(β -(3,4-diethoxyphenyl)ethyl)galloylamine tri-Me ether (X), C₂₂H₂₉O₆N, m. 130-1°, colorless bright needles. X (5 g.) in toluene (15 cc.) and POCl₃ (9 g.) on boiling 2 hrs. gave 1 - (3',4',5' - trimethoxyphenyl) - 6,7 - diethoxy - 3,4-dihydroisoquinoline (XI), C₂₂H₂₇O₅N, m. 163-4° (yield 2 g.). XI (2 g.) in xylene (15 cc.) and Pd black (0.5 g.) on heating for 3 hrs. at 150° gave 1-(3',4',5'-trimethoxy-phenyl)-6,7-diethoxyisoquinoline, C₂₂H₂₅O₅N, m. 117-18° (yield 1.1 g.).

IT 872270-11-6P, Isoquinoline,
6,7-diethoxy-1-(3,4,5-trimethoxyphenyl)-
RL: PREP (Preparation)

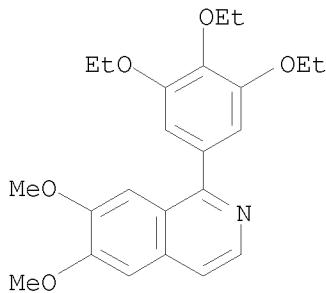
(preparation of)

RN 872270-11-6 HCPLUS

CN Isoquinoline, 6,7-diethoxy-1-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 305 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1934:37242 HCPLUS
 DOCUMENT NUMBER: 28:37242
 ORIGINAL REFERENCE NO.: 28:4476g-h
 TITLE: Octaverin, a new substance causing paralysis of smooth muscle
 AUTHOR(S): Ellinger, Ph.; Koschara, W.; Seeger, H.
 SOURCE: Klinische Wochenschrift (1934), 13, 411
 CODEN: KLWOAZ; ISSN: 0023-2173
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB A preliminary report. The substance is 1 - (3,4,5-triethoxyphenyl) - 6,7 - dimethoxyisoquinoline.
 IT 549-68-8P, Octaverine
 RL: PREP (Preparation)
 (preparation of)
 RN 549-68-8 HCPLUS
 CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



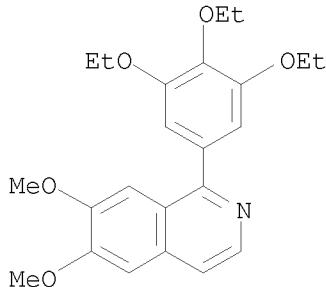
L13 ANSWER 306 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1934:34922 HCPLUS
 DOCUMENT NUMBER: 28:34922
 ORIGINAL REFERENCE NO.: 28:4178h-i, 4179a-c
 TITLE: Synthetic drugs
 PATENT ASSIGNEE(S): I. G. Farbenindustrie AG
 SOURCE: Addn. to 377,255 (C. A. 27, 4032)
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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GB 404674		19340119	GB 1932-20456	19320719 <--

AB Therapeutically valuable compds. are prepared by combining the N atom of an amine of the formula NHRR' (where R and R' are 2 identical or different univalent hydroaromatic hydrocarbon residues which may be bound to each other by a CH₂ group, or 2 identical or different hydroaromatic-aliphatic hydrocarbon residues) by means of an aliphatic residue with a N atom of a pyridine or quinoline compound containing a tautomeric amino group. Suitable amines of the above formula are dicyclohexylamine (I), perhydroacridine (II), dihexahydrobenzylamine, dicyclohexylethylamine and cyclohexylhexahydrobenzylamine (obtainable by interaction of hexahydrobenzylamine with cyclohexyl bromide). Among examples (1) I is treated with ethylene chlorohydrin, the resulting β-dicyclohexylaminoethanol converted by means of SOC₁₂ into β-dicyclohexylaminoethyl chloride and the latter combined with 2-aminopyridine (III), 2-aminoquinoline or the Na compound of III to give 1-dicyclohexylaminoethyl-2-iminopyridine, 1-dicyclohexylaminoethyl-2-iminoquinoline or 2-dicyclohexylaminoethylaminopyridine, resp.; (2) II, prepared by hydrogenating acridine in a solvent with a Ni catalyst, is treated with ethylene chlorohydrin and then with SOC₁₂ and the resulting chloroethylperhydroacridine combined either with III to form 1-perhydroacridylethyl-2-iminopyridine or with 6-ethoxy-4-aminoquinaldine to give 1-perhydroacridylethyl-2-methyl-6-ethoxy-4-iminoquinoline; and (3) 1-(1'-dicyclohexylamino-4'-pentyl)-2-iminopyridine is obtained by interaction of III with 1-dicyclohexylamino-4-pentyl chloride, obtained from 1-dicyclohexylamino-4-pentanol (IV) and SOC₁₂; IV is obtained by heating β-dicyclohexylaminoethyl chloride with EtOAc and then with AcOH and reducing the resulting ketone with H in presence of Ni.

STN

IT 549-68-8P, Octaverine
RL: PREP (Preparation)
(preparation of)
RN 549-68-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



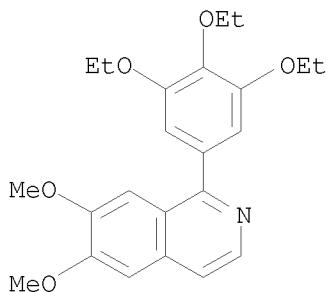
L13 ANSWER 307 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1934:34921 HCPLUS
DOCUMENT NUMBER: 28:34921
ORIGINAL REFERENCE NO.: 28:4178g-h
TITLE: Therapeutic compounds
PATENT ASSIGNEE(S): Asta A.-G. Chemische Fabrik
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 760825		19340303	FR	19330829 <--

AB 1-(3',4',5'-trialkoxyphenyl)-6,7-dialkoxyisoquinolines are prepared by treating the β -dialkylphenyl- β -methoxyethylamides of trialkylgallic acids by acid condensing agents in indifferent organic solvents, preferably halogenated hydrocarbons, using at most 4 times the theoretical amount of condensing agent and causing it to arrive drop by drop in the boiling solution of acid amide. Examples are given of the preparation of the HCl compound of (1) the triethoxy-dimethoxy, m. 217° with decomposition, (2) the trimethoxy-dimethoxy, m. 199-200°, and (3) the triethoxy-methylenedioxy (m. 283-5° with decomposition) compds. The products may replace papaverine and known phenylisoquinolines in therapeutics.

IT 549-68-8P, Octaverine
RL: PREP (Preparation)
(preparation of)
RN 549-68-8 HCPLUS
CN Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 308 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1934:14069 HCPLUS

DOCUMENT NUMBER: 28:14069

ORIGINAL REFERENCE NO.: 28:1703c-e

TITLE: Isoquinoline derivatives. III.
3-Isoquinolinecarboxylic acids

AUTHOR(S): Harwood, H. J.; Johnson, T. B.

SOURCE: Journal of the American Chemical Society (1934
(1934), 56, 468-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 27, 5743. The Me ester, m. 143-4°, and the Et ester, m. 118-19°, of α -benzamido-3,4-dimethoxycinnamic acid, on catalytic reduction give the Me ester, m. 104-5°, and the Et ester, m. 100-1°, of N-benzoyl-3,4-dimethoxyphenylalanine; these esters with P205 in boiling xylene give the Me ester, m. 120.5-1.5°, and the Et ester, resp., of 1-phenyl-6,7-dimethoxy-3,4-dihydro-3-isooquinolinecarboxylic acid (I). I with SOCl_2 and MeOH gives Me 1-phenyl-6,7-dimethoxy-3-isooquinolinecarboxylate, m. 172-3°; the free acid, m. 216-6.5°; I with PCl_5 in C_6H_6 gives an acid chloride, which regenerates the Me ester of I with MeOH . Heating I in C_6H_6 causes decarboxylation, giving 1-phenyl-6,7-dimethoxy-3,4-dihydroisoquinoline (II), m. 120.5-1.5°, identical with that obtained by the ring closure of N-(3,4-dimethoxyphenylethyl)benzamide, m. 90-1°, prepared from homoveratrylamine and BzCl in 10% NaOH . The chloride from I and SOCl_2 with $\text{Et}_2\text{NCH}_2\text{CH}_2\text{OH}$ gives the diethylaminoethyl ester of II, m. 158.5-9°.

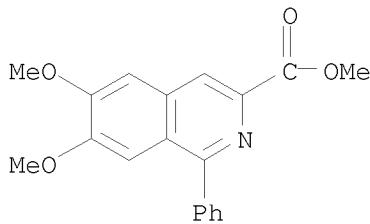
IT 1071579-43-5P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Isoquinoline derivatives. III. 3-Isoquinolinecarboxylic acids)

RN 1071579-43-5 HCPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-phenyl-, methyl ester (CA INDEX NAME)

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OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

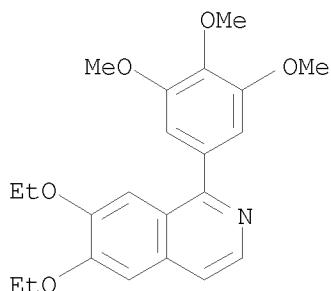
L13 ANSWER 309 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1934:8822 HCPLUS
DOCUMENT NUMBER: 28:8822
ORIGINAL REFERENCE NO.: 28:1103e-g
TITLE: Antispasmodics of the papaverine type
AUTHOR(S): Slotta, K. H.; Haberland, G.
SOURCE: Angewandte Chemie (1933), 46, 766-71
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Three β -arylethylamines, 2 alkoxybenzoic acids and nine 1-phenylisoquinolines were prepared; the latter were obtained by reaction of the first 2 kinds of compds. The pharmacol. tests of the 1-phenylisoquinolines showed that the size and number of the alkoxy groups in the mol. are of great importance. If 5 methoxyl groups are present the compound in nontoxic quantities has a paralyzing action upon smooth muscle tissue. Introduction of 2 ethoxyl and 3 methoxyl groups greatly increases the action, but a decrease occurs when 5 ethoxyl groups are present and the action disappears with 6 methoxyl groups. The most effective compound prepared so far is the 1-(3', 4', 5'-trimethoxyphenyl)-6,7-diethoxyisoquinoline which was examined and compared with papaverine and atropine. The lethal dose and the action upon the stomach and the small and large intestine were determined for these substances. Exptl. data are presented for all substances which were prepared Thirty-one references.

IT 872270-11-6, Isoquinoline,
6,7-diethoxy-1-(3,4,5-trimethoxyphenyl)-
(antispasmodic action of)

RN 872270-11-6 HCPLUS

CN Isoquinoline, 6,7-diethoxy-1-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)



L13 ANSWER 310 OF 310 HCPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1927:13497 HCPLUS
DOCUMENT NUMBER: 21:13497
ORIGINAL REFERENCE NO.: 21:1655a-f
TITLE: Experiments in the isoquinoline series and synthesis
of papavarine
AUTHOR(S): Rosenmund, K. W.; Nothnagel, Margarethe; Riesenfeldt,
Hermine
SOURCE: Berichte der Deutschen Chemischen Gesellschaft
[Abteilung] B: Abhandlungen (1927), 60B,
392-8
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Only py-hydrogenated isoquinolines are readily obtained by the Pictet and Decker method, as there are no easily available starting materials for the preparation of the non-hydrogenated compds. R., N. and R. thought the desired object might be attained by dehydrating ω -phenylvinylamines but they were no more successful than other workers in preparing such amines by the method according to which Komopa thought he obtained PhCH:CHNH₂, at least in Et₂O solution (Ber. 26, 677(1893)), and either they are not capable of existence or are so sensitive that they change very rapidly under even mild conditions. In the hope that their acyl derivs. would be more stable, a number of phthalyl and Bz derivs. were prepared from bromostyrenes with C₆H₄(CO)₂NK and BzNH₂ in the presence of K₂CO₃ and a little Cu, but like the unacylated amines they also undergo undesirable changes under the conditions necessary to undergo ring closure. Finally, it was found that Al₂O₃ is a sufficiently mild dehydrating agent to bring about the desired reaction, but unfortunately this action is greatly dependent on the nature of the Al₂O₃ and of many samples at hand only a few proved effective; moreover, in spite of many efforts, it has not been possible to devise a reliable method for obtaining efficient preps. The acyl derivs. of the β -alkoxy- β -phenylethylamines, readily obtained from the nitrostyrenes with Na alcoholates, followed by reduction, condense, however, to the desired isoquinolines with P2O5.
N-Phthalyl- ω -phenylvinylamine (N-styrylphtalimide) (yield, 60.37%). yellow. m. 188-9°; HBr addition product, m. 107-8° (vigorous evolution of HBr). Alc. KOH hydrolyzes the imide to the phthalamidic acid, yellow, m. 169°. PhCH:CHNH₂ (I), m. 174-5° (Komppa gives 161°). N-Benzoyl- ω -[3,4-methylenedioxyphenyl]vinylamine, m. 159°.
N-Benzoyl- ω [4-methoxyphenyl]vinylamine, faintly yellow, m. 169°. From I in boiling decalin treated with 20 parts Al₂O₃ (dried at 400°) in small portions and boiled 6-7 hrs. was obtained 1-phenylisoquinoline. α -[3,4-Dimethoxyphenyl]- ω -nitroethanol Me ether (14-5 g. from (MeO)₂C₆H₃CH:CHNO₂ in MeOH with NaOMe at 15°). m. 106°. α -[3,4-Methylenedioxy] analog, light yellow, m. 62°. (MeO)₂C₆H₃CH(OMe)CH₂NH₂ (II), from the NO₂ compound in MeOH with AcOH and Na-Hg, b13 170° (HCl salt, m. 185°; Bz derivative, m. 124°). β -[3,4-Methylene-dioxyphenyl] analog; HCl salt, m. 162°. The Bz derivative of II with P2O5 in boiling Xylene gives 1-phenyl-6,7-dimethoxyisoquinoline, isolated as the picrate, m. 250°. II with 3,4-(MeO)₂C₆H₃CH₂COCl gives the acid amide (MeO)₂C₆H₃CH(OMe)CH₂NHCOCH₂C₆H₃(OMe)₂, m. 147-8°, 2 g. of which with P2O5 in xylene yield 0.13 g. of papaverine, m. 182-3°. This

STN

paper was read at the Versammlung Deutscher Naturforscher und Arzte in Dusseldorf, where Mannich reported he had obtained similar and better results with POC13 as the condensing agent.

IT 4029-09-8P, Isoquinoline, 6,7-dimethoxy-1-phenyl-

RL: PREP (Preparation)
(preparation of)

RN 4029-09-8 HCPLUS

CN Isoquinoline, 6,7-dimethoxy-1-phenyl- (CA INDEX NAME)

